
The 36-th Conference
of the Middle European Cooperation
in Statistical Physics
5-7 April 2011, Lviv, Ukraine
MECO 36
PROGRAMME AND ABSTRACTS

The 36-th Conference of the Middle European Cooperation in Statistical Physics

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PROGRAMME AND ABSTRACTS

Lviv – 2011

Organizer

Institute for Condensed Matter Physics
of the National Academy of Sciences of Ukraine
Lviv, Ukraine

Co-organizers

Ivan Franko National University
of Lviv, Ukraine

Lviv Polytechnic National
University, Ukraine

Sponsors

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Contacts

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Previous MECO conferences

2010 Pont-á-Mousson (F)
2009 Leipzig (D)
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2004 Bratislava (SK)
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1987 Poidoux-Chexbres (CH)
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1982 Wien (A)
1981 Saarbrücken (D)
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1978 Boszkowo (PL)
1977 Unterägeri (CH)
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1975 Regensburg (D)
1974 Wien (A)

Preface

In the middle of the 1970's, the European physics community initiated a series of international conferences, called the Middle European Cooperation in Statistical Physics (MECO). This initiative very soon spread over Europe in a wider sense, covering not only the middle-European countries.

During the last two decades of the Cold War, the conference series allowed statistical physicists in the East and West to maintain open scientific dialogue and beneficial collaborations across the iron curtain. Since their establishment, the MECO conferences became one of the most prestigious forums in statistical physics and related disciplines. In more recent times, due to interdisciplinary applications, MECO attracts the attention of a much wider academic community.

The 36th MECO conference is planned to continue this tradition. It will be held on the 5th – 7th of April in the city of Lviv, main cultural, academic and political center in western Ukraine. The Conference is organized in the form of invited lectures (about 40 min.), oral contributions (about 20 min.) and poster presentations. The scope of the conference covers different fields of statistical mechanics and condensed matter physics with special emphasis on such topics as soft matter, complex systems and networks, non-equilibrium systems, and spin models.

More than 150 attendees from 22 countries are expected for MECO 36. We warmly welcome you in the city of Lviv and thank you for registering for the conference. May future MECO by our common efforts become an interesting and enjoyable meeting!

MECO 36 local organizers

The 36-th Conference
of the Middle European Cooperation in Statistical Physics

Programme

5–7 April 2011, Lviv, Ukraine

Monday, 4 April, 2011

14.00 – 18.00	Registration	*Lviv Polytechnic National University, 1st floor, room 226 (12 St. Bandera Street)*
19.00 – 22.00	Welcome party	*Будинок вчених House of Scientists (6 Lystopadovoho chynu Street)*

Tuesday, 5 April, 2011

Lviv Polytechnic National University, Mateyko Hall

09.10 – 09.20 Welcome

Chaired by Ihor Mryglod *(Lviv, Ukraine)*

09.20 – 10.00 Yoseph Imry *(Rehovot, Israel)*
Slow relaxation and aging in electron glasses distance matrix description *(Invited lecture)*

10.00 – 10.20 Leticia Cugliandolo *(Paris, France)*
Cooling rate dependencies across thermal phase transitions

10.20 – 10.40 Oleksandr Bakai *(Kharkiv, Ukraine)*
Thermodynamics of structured amorphous states: fluid, liquid, glass

10.40 – 11.10 Coffee

Lviv Polytechnic National University, Room 210

Chaired by Wolfhard Janke *(Leipzig, Germany)*

11.10 – 11.50 Gerhard Kahl *(Wien, Austria)*
***Predicting* ordered equilibrium structures for patchy particles** *(Invited lecture)*

11.50 – 12.10 Antonio Scala *(Roma, Italy)*
Patchy depletion interactions

12.10 – 12.30 Ivo Nezbeda *(Usti n. Labem, Czech Republic)*
Generalized excluded volume: its origin and effects

12.30 – 14.00 Lunch

14.00 – 15.30 Poster session
(odd numbers of the list on pp. 21–31)

Chaired by: Christian von Ferber *(Coventry, England)*
Yurij Kalyuzhnyi *(Lviv, Ukraine)*
Stefan Sokolowski *(Lublin, Poland)*
Yulian Vysochanskii *(Uzhgorod, Ukraine)*
Tomasz Wydro *(Nancy, France)*

Lviv Polytechnic National University, Room 210

Chaired by Bertrand Berche *(Nancy, France)*

15.30 – 16.10 Helena Zapolsky *(Rouen, France)*
From atomistic to mesoscale description of phase transitions *(Invited lecture)*

16.10 – 16.30 Wolfhard Janke *(Leipzig, Germany)*
Worms exploring geometrical features of phase transitions

16.30 – 16.50 Alexander Chalyi *(Kyiv, Ukraine)*
Diffusion phenomena in confined liquids near the critical point

16.50 – 17.20 Coffee

Lviv Polytechnic National University, Room 210

Chaired by Krystyna Lukierska-Walasek
(Zielona Góra, Poland)

17.20 – 17.40 Pascal Viot *(Paris, France)*
Heterogeneous granular motors

17.40 – 18.00 Arnaldo Donoso *(Caracas, Venezuela)*
A brief review on energy recycling from thermal fluctuations

18.00 – 18.20 Giuseppe Gonnella *(Bari, Italy)*
Self-propelled particles under shear

19.00 Dinner

Wednesday, 6 April, 2011

Lviv Polytechnic National University, Room 210

Chaired by Frantisek Slanina *(Prague, Czech Republic)*

09.20 – 10.00 José Fernando Mendes *(Aveiro, Portugal)*
Bootstrap percolation on complex networks *(Invited lecture)*

10.00 – 10.20 Reinhard Mahnke *(Rostock, Germany)*
Power laws and skew distributions

10.20 – 10.40 Ralph Kenna *(Coventry, England)*
Critical mass and the dependency of research quality on group size

10.40 – 11.10 Coffee

Lviv Polytechnic National University, Room 210

Chaired by Oksana Patsahan *(Lviv, Ukraine)*

11.10 – 11.50	Clemens Bechinger *(Stuttgart, Germany)* **The force of fluctuations** *(Invited lecture)*	
11.50 – 12.30	Andrea Gambassi *(Trieste, Italy)* **Steering the critical Casimir effect: lateral forces, levitation, and dynamics** *(Invited lecture)*	
12.30 – 12.50	Oleg Vasilyev *(Stuttgart, Germany)* **Critical Casimir forces for various boundary fields obtained by Monte Carlo simulation: crossover from repulsion to attraction**	
12.50 – 14.30	Lunch	
15.00	Excursion	
19.00	Conference Dinner	*Ресторан "Високий Замок"* *Restaurant "Vysokyi Zamok"*

Thursday, 7 April, 2011

Lviv Polytechnic National University, Room 210

Chaired by Reinhard Folk *(Linz, Austria)*

09.20 – 10.00 Alina Ciach *(Warsaw, Poland)*
Mesoscopic theory for inhomogeneous mixtures
(Invited lecture)

10.00 – 10.20 Dominique Mouhanna *(Paris, France)*
Nonperturbative renormalization group approach to polymerized membranes

10.20 – 10.40 Jozef Strečka *(Košice, Slovak Republic)*
Weak-universal critical behavior in the exactly solved mixed-spin Ising model with the triplet interaction on a centered square lattice

10.40 – 11.10 Coffee

Lviv Polytechnic National University, Room 210

Chaired by Yurii Slyusarenko *(Kharkiv, Ukraine)*

11.10 – 11.30 Józef Sznajd *(Wrocław, Poland)*
On the search for a Lifshitz point in UPd_2Si_2

11.30 – 11.50 Oleh Velychko *(Lviv, Ukraine)*
Thermodynamics and dynamics of the two-state Bose-Hubbard model in the effective pseudospin representation

11.50 – 12.10 Daniel Cabra *(La Plata, Argentina)*
Anharmonic effects in magnetic systems

12.10 – 12.30 Tadeusz Domanski *(Lublin, Poland)*
Residual diamagnetism driven by the superconducting fluctuations

12.30 – 14.00 Lunch

14.00 – 15.30 Poster session
(even numbers of the list on pp. 21–31)

Chaired by: Christian von Ferber *(Coventry, England)*
Yurij Kalyuzhnyi *(Lviv, Ukraine)*
Stefan Sokolowski *(Lublin, Poland)*
Yulian Vysochanskii *(Uzhgorod, Ukraine)*
Tomasz Wydro *(Nancy, France)*

Lviv Polytechnic National University, Room 210

Chaired by Józef Sznajd *(Wrocław, Poland)*

15.30 – 16.10 Aleksei Chechkin
(Kharkiv, Ukraine/Tel Aviv, Israel)
A few "paradoxes" of Lévy flights *(Invited lecture)*

16.10 – 16.30 Gleb Oshanin *(Paris, France)*
Dynamics in disordered media: Applications to biophysics, mathematical finance and etc.

16.30 – 16.50 Aleksander Stanislavsky *(Kharkiv, Ukraine)*
Subdiffusion with a time-dependent force: the case of under- and overshooting subordination

16.50 – 17.20 Coffee

Lviv Polytechnic National University, Room 210

Chaired by Anton Šurda *(Bratislava, Slovak Republic)*

17.20 – 17.40 Alexey Savin *(Saratov, Russia)*
The critical behavior of Hamiltonian type in driven and coupled dissipative systems

17.40 – 18.00 Leonardo Banchi *(Sesto Fiorentino, Italy)*
Efficient quantum information transfer through a uniform channel

18.00 – 18.20 Tony J.G. Apollaro *(Sesto Fiorentino, Italy)*
Manipulating and protecting entanglement by means of spin environments

18.20 Closing

19.00 Dinner

LIST OF POSTERS

The awards for six best conference posters will be introduced. Among these six posters, three posters will be selected by the jury of the poster session chairs and the other three by the participants of the conference. In the latter case each participant will have several sticky markers, which can be used to mark the poster he/she likes. Three posters, which will collect the largest number of the markers, and three posters, selected by the jury, will be awarded.

1. Andrusyk A. *(Lviv, Ukraine)*
   Piezoelectric resonance in Rochelle salt

2. Baran O.R. *(Lviv, Ukraine)*
   Phase diagrams of spin-3/2 Blume-Capel model on rectangular lattice under longitudinal magnetic field

3. Belyi V.V. *(Troitsk, Russia)*
   Non-Markov kinetic equation for quantum plasma with exchange interaction

4. Blavatska V. *(Lviv, Ukraine)*
   Shape anisotropy of polymers in porous environment

5. Bose T. *(Halle, Germany)*
   Noise and retardation effects in the Landau-Lifshitz-Gilbert equation

6. Burmistrov I. *(Moscow, Russia)*
   Spin and charge correlations in quantum dots: an exact solution

7. Bzovska I. *(Lviv, Ukraine)*
   Bistability and oscillatory behavior in heterogeneous catalysis: CO oxidation reaction

8. Chepizhko O.O. *(Odessa, Ukraine)*
   The kinetics of the order-disorder transition in the models of dynamic synchronization

9. Derzhko O. *(Lviv, Ukraine)*
Exactly solvable random spin-$\frac{1}{2}$ XX chain with three-site interactions

10. Dubrovskiy I. *(Kyiv, Ukraine)*
Statistical mechanics of rotating gas

11. Ekiz C. *(Aydın, Turkey)*
Exact results of the mixed spin-1/2 and spin-1 Ising model on a decorated Bethe lattice

12. Emelianova Yu. *(Saratov, Russia)*
Non-identity in system of coupled elements

13. Erdem R. *(Antalya, Turkey)*
Static quadrupolar susceptibility for the Blume-Emery-Griffiths Model

14. Dublenych Yu.I. *(Lviv, Ukraine)*
Structures on lattices: Some useful relations

15. Folk R. *(Linz, Austria)*
Localization transition in binary mixture with high mass asymmetry

16. Fricke N. *(Leipzig, Germany)*
A new technique for complete enumeration of self-avoiding walks (SAWs) on percolation clusters

17. Gerasimenko V.I. *(Kyiv, Ukraine)*
On quantum kinetic evolution of marginal observables

18. Grytskiv R. *(Lviv, Ukraine)*
A molecular dynamics study of collective dynamics in a binary glass

19. Gubceac G. *(Chisinau, Moldova)*
Impact of asymmetry on phase transitions in the presence of an intermediate metastable state

20. Haydukivska K. *(Lviv, Ukraine)*
Conformational transitions in semiflexible polymers

21. Hlushak S. *(Lviv, Ukraine/Paris, France)*
Modelling speciation in nitric acid solutions using the Associative Mean Spherical Approximation

22. Holovatch T. *(Nancy, France/Coventry, England)*
Exploration of a radial bus system: Modelling and optimisation

23. Hucht A. *(Duisburg, Germany)*
Aspect-ratio dependence of thermodynamic Casimir forces

24. Humenyuk Y.A. *(Lviv, Ukraine)*
Transport coefficients of a dense fluid mixture with multistep interaction between particles

25. Ignatyuk V.V. *(Lviv, Ukraine)*
Coherence, decoherence, and memory effects in the problems of quantum surface diffusion

26. Ilnytskyi J.M. *(Lviv, Ukraine)*
Computer simulation of a self-assembly of liquid crystalline dendrimers

27. Ivaneyko D. *(Dresden, Germany)*
Magneto-sensitive elastomers in a homogeneous magnetic field: a regular rectangular lattice model

28. Juhász R. *(Budapest, Hungary)*
Dynamics at barriers in bidirectional two-lane exclusion processes

29. Kalyuzhnyi Yu. *(Lviv, Ukraine)*
Resummed thermodynamic perturbation theory for central force associating potential. Multi-patch models

30. Kaupužs J. *(Riga/Liepaja, Latvia)*
Power laws and critical exponents in n-vector models

31. Kavalets I.I. *(Lviv, Ukraine)*
Gini index for measuring the statistical heterogeneity

32. Kharchenko D.O. *(Sumy, Ukraine)*
Stochastic effects at pattern formation processes during ion-beam sputtering

33. KLEVETS I. *(Lviv, Ukraine)*
Features of dynamical properties of liquid polyvalent metals near melting point: ab initio molecular dynamics study

34. KOSTROBIJ P.P. *(Lviv, Ukraine)*
Chemical potential of semi-infinite jellium

35. KOVÁCS I.A. *(Budapest, Hungary)*
Entanglement entropy of the random transverse-field Ising model in higher dimensions

36. KOZAK P.R. *(Lviv, Ukraine)*
The equation of state of the n-vector model

37. KOZITSKY YU. *(Lublin, Poland)*
Quenched thermodynamic states of the Ising model on random graphs

38. KRAMAR O. *(Ternopil, Ukraine)*
Ferromagnetism in spin subsystem hybridized with conduction band in Anderson-Hubbard-type model

39. KRAVTSIV I. *(Lviv, Ukraine)*
Field theoretical approach for a nematic fluid: beyond the Maier-Saupe theory

40. KRIVNOV V.YA. *(Moscow, Russia)*
Low-temperature properties of frustrated classical spin chain near the ferromagnet-helimagnet transition point

41. KROKHMALSKII T. *(Lviv, Ukraine)*
Magnetization processes at low temperatures for two frustrated quantum Heisenberg antiferromagnets

42. KULINSKII V.L. *(Odessa, Ukraine)*
Global isomorphism between the Lennard-Jones fluids and the Ising model

43. KUPOROV V.M. *(Lviv, Ukraine)*
Mutual diffusion and partial conductivities in multicomponent ionic liquids

44. Kurzidim J. *(Wien, Austria)*
Slow dynamics of colloids in porous media: the roles of confinement and caging

45. Levitskii R.R. *(Lviv, Ukraine)*
Dielectric, piezoelectric and elastic properties of quasione-dimensional $Cs(H_{1-x}D_x)_2PO_4$ ferroelectrics

46. Lisnii B.M. *(Lviv, Ukraine)*
Spin-1/2 asymmetrical diamond Ising-Heisenberg chain

47. Lukierska-Walasek K. *(Zielona Góra, Poland)*
Everything about statistics of the Ising model

48. Mac Carron P. *(Coventry, England)*
Networks in mythology

49. Magiera M.P. *(Duisburg, Germany)*
Magnetic friction – from Stokes to Coulomb

50. Mahlaichuk P. *(Odessa, Ukraine)*
Contribution of H-bond vibrations to the heat capacity of water

51. Maksymenko M. *(Lviv, Ukraine)*
Localized states on triangular traps and low-temperature properties of some strongly correlated lattice models

52. Maksymenko M. *(Lviv, Ukraine)*
Transition to ferromagnetic ground-states in the two-dimensional Tasaki-Hubbard model

53. Markiv B.B. *(Lviv, Ukraine)*
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54. Matskevych V.T. *(Kharkov, Ukraine)*
Biaxial nematic liquid crystals: Green functions and polarization features of acoustic waves

55. Melnyk R. *(Lviv, Ukraine)*
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56. Möddel M. *(Leipzig, Germany)*
Comparison of grafted and non-grafted polymer adsorption in different ensembles

57. Moina A.P. *(Lviv, Ukraine)*
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58. Mryglod O. *(Lviv, Ukraine)*
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59. Mysakovych T.S. *(Lviv, Ukraine)*
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60. Najafi M.N. *(Tehran, Iran)*
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64. Parisen Toldin F. *(Dresden, Germany)*
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65. Patsahan O.V. *(Lviv, Ukraine)*
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66. Pavlenko N. *(Lviv, Ukraine)*
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67. Pešek J. *(Prague, Czech Republic)*
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68. Pizio O. *(Coyocan, Mexico)*
Structural and thermodynamical properties of the restricted primitive model electrolyte in a mixture with uncharged hard-spheres. A grand canonical Monte Carlo simulation and hnc integral equation study

69. Pizio O. *(Coyocan, Mexico)*
Adsorption of a solvent primitive model for electrolyte solutions in disordered porous matrices of charged species. Replica Ornstein-Zernike theory and grand canonical Monte Carlo simulations

70. Pokorný V. *(Prague, Czech Republic)*
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71. Polishchuk D.O. *(Kiev, Ukraine)*
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72. Pylyuk I.V. *(Lviv, Ukraine)*
Method of calculating the free energy of a 3D Ising-like system taking into account the correction for the interaction potential averaging

73. Romanik R.V. *(Lviv, Ukraine)*
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74. Rżysko W. *(Lublin, Poland)*
Phase behavior of heteronuclear rigid trimers

75. Sakhnyuk V.E. *(Lutsk, Ukraine)*
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76. Scala A. *(Roma, Italy)*
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77. Shchur Ya. *(Lviv, Ukraine)*
Lattice dynamics model of hydrogen-bonded crystals of KH_2PO_4-type

78. Shmotolokha V. *(Lviv, Ukraine)*
Hard convex body fluids in random porous media

79. Shpot M.A. *(Lviv, Ukraine)*
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80. Shvets V.T. *(Odesa, Ukraine)*
Equation of state for extrasolar giant planets

81. Shvets V.T. *(Odesa, Ukraine)*
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82. Shygorin P.P. *(Lutsk, Ukraine)*
Sounds in the dilute condensed Bose-gas

83. Slanina F. *(Prague, Czech Republic)*
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Two approaches to description of fractional Brownian motion

85. Slyusarenko Yu.V. *(Kharkiv, Ukraine)*
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86. Sokolovsky A.I. *(Dnipropetrovs'k, Ukraine)*
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87. Sokolovsky S.A. *(Dnipropetrovs'k, Ukraine)*
To phonon hydrodynamics in crystalline solid

88. Sokołowski S. *(Lublin, Poland)*
Density functional theory of adsorption on surfaces modified with tethered brushes

89. Sorokov S.I. *(Lviv, Ukraine)*
Longitudinal dielectric, piezoelectric and elastic properties of the $K_{1-x}(NH_4)_xH_2PO_4$ type mixed crystals. Simple model

90. Stetsiv R.Ya. *(Lviv, Ukraine)*
Dielectric and superfluid-like states of one-dimensional ionic Pauli conductor

91. Stetsiv R.Ya. *(Lviv, Ukraine)*
Dynamic properties of quasi-one-dimensional structures with hydrogen bonds

92. Strečka J. *(Košice, Slovak Republic)*
Thermodynamic properties of the spin-1/2 Ising-Heisenberg model on a triangle-hexagon lattice

93. Stupka A.A. *(Dnipropetrovs'k, Ukraine)*
Hydrodynamic modes in external fluctuating field

94. Šurda A. *(Bratislava, Slovak Republic)*
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95. Taloni A. *(Tel Aviv, Israel)*
Generalized elastic models: fractional dynamics representation and beyond

96. Tokarchuk M.V. *(Lviv, Ukraine)*
Nonequilibrium statistical operator method in Renyi statistics

97. Topilko M. *(Lviv, Ukraine)*
Magnetocaloric effect and magnetic cooling in the spin-$\frac{1}{2}$ XX chain with three-site interactions

98. Topilko M. *(Lviv, Ukraine)*
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99. Trokhimchuck P.P. *(Lutsk, Ukraine)*
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100. Trokhymchuk A. *(Lviv, Ukraine)*
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101. Tsvir Zh.A. *(Kyiv, Ukraine)*
Generalized quantum kinetic equation for interacting particles with quantum statistics

102. Usatenko Z. *(Lviv, Ukraine)*
Universal amplitude in density-force relations for polymer chains in confined geometries

103. Vaia R. *(Sesto Fiorentino, Italy)*
Time dependent spread of a generic 1D wavepacket

104. Vasylenko A.I. *(Lviv, Ukraine)*
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105. Vasylenko A.I. *(Lviv, Ukraine)*
Statistical description of electrodiffusion processes in the electron subsystem of a semibounded metal within the generalized jellium model

106. Verkholyak T. *(Lviv, Ukraine)*
The two-component BCSOS model of surface as a dimerized quantum spin-1/2 chain

107. von Ferber C. *(Coventry, England/Freiburg, Germany)*
Star copolymers in porous environments: scaling and its manifestations

108. Vysochanskii Yu.M. *(Uzhgorod, Ukraine)*
Theoretical prediction and experimental evidence of Blume-Emery-Griffiths phase diagram in the uniaxial $Sn_2P_2S_6$ ferroelectrics

109. Weber H. *(Luleå, Sweden)*
Latent heat of a traffic model

110. Wydro T. *(Nancy, France)*
Lattice model of liquid crystalline structures with spontaneously broken chiral symmetry

111. Yanishevsky V.S. *(Drohobych, Ukraine)*
Use methods of statistical physics in optimization problems

112. Zaburannyi O. *(Lviv, Ukraine)*
Strong-interaction approximation for transfer-matrix method

113. ZACHEK I.R. *(Lviv, Ukraine)*
Longitudinal and transverse dielectric, piezoelectric, elastic, dynamic, and thermal properties of the Rochelle salt $NaKC_4H_4O_6 \cdot 4H_2O$

114. ZADVORNYAK I.M. *(Lviv, Ukraine)*
Two-particle electron correlation function of semi-infinite jellium

115. ZHILENKO T.I. *(Sumy, Ukraine)*
Investigation of hierarchical condensation conditions near phase equilibrium

The 36-th Conference
of the Middle European Cooperation in Statistical Physics

Invited Lectures

Abstracts

5–7 April 2011, Lviv, Ukraine

Slow relaxation and aging in electron glasses distance matrix description

Y. Imry

CM Physics, the Weizmann Institute

(Based on work with Ariel Amir and Yuval Oreg)

The phenomena of slow relaxation and "aging" in glasses, with emphasis on electronic ones, will be briefly reviewed. It will be shown that a spectrum of relaxation rates, λ, behaving approximately as $1/\lambda$ (for small λ) can explain these effects, while producing a universal description in terms of a simple function. We find that this description holds also for other glasses and for different physical properties. We obtained this spectrum before, based on approximations for the hopping model. Now we shall consider the related random "distance" matrices model, where the matrix elements depend exponentially on the distance between uniformly and randomly distributed points. This model arises naturally in various further physical contexts, such as the diffusion of particles, and scalar phonon localization. Using a combination of a renormalization group procedure and a direct moment calculation, we find the exact eigenvalue distribution and the localization properties of the eigenmodes, at low densities, for **arbitrary dimension**. The results agree perfectly with numerics. Finally, we discuss the physical implications of the results vis a vis the universal relaxation mentioned above. We shall show that much of the relevant Physics is captured by this model.

Predicting ordered equilibrium structures for patchy particles

G. Kahl

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From the basic laws of thermodynamics we know that for given external parameters, such as pressure or temperature, particles will always arrange in ordered equilibrium structures such that the respective thermodynamic potential is minimized with respect to the lattice parameters that define the structure. However, in practice this minimization task turns out to be highly non-trivial and from the numerical point of view very delicate: high dimensional parameter spaces and rugged energy landscapes are the main problems that have to be faced. A few years ago we have proposed an optimization strategy that is based on ideas of genetic algorithms. In this concept, a possible ordered structure is considered to be an individual that is exposed on the computer to some artificial evolution: in this process the individuals have to survive under the condition that their thermodynamic potential is as small as possible. In this way, the individuals 'converge' after a reasonable number of generations towards the equilibrium structure. In subsequent numerous applications to a large variety of soft matter systems we have found that this optimization strategy is highly flexible, reliable, and efficient and that it copes extremely well with the above mentioned problems.

In this contribution we will discuss ordered equilibrium structures formed by so-called patchy particles, i.e., spherically symmetric colloids that are decorated on their surface by mutually repelling and/or attracting regions. Very recently, such particles have attracted the attention of soft matter scientists: experimentalists are now able to locate the patchy regions with high precision on the colloidal surface and to neatly define their spatial extent. With their highly directional potentials, these patchy particles are therefore excellent candidates to form ordered equilibrium structures with a desired symmetry. Our extensive investigations based on the genetic algorithm technique provides some insight into the self-assembly strategy of patchy particles.

From atomistic to mesoscale description of phase transitions

H. Zapolsky
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Although the present understanding of atomic systems in thermodynamic equilibrium is rather satisfactory and is based on well established theoretical methods, the dynamic theory of atomic-scale evolution during phase transformation is far from completion in spite of extensive experimental and theoretical investigations. The highly nonlinear and nonequilibrium dynamics of phase transformations at mesoscale have been extensively studied by employing continuum Ginzburg-Landau-Khalatnikov (Phase Field) or Cahn-Hilliard-type kinetic equations. With random thermal noises, both types of equations become stochastic, and their applications to studying critical dynamics have been extensively discussed. During the past ten years, the phase-field approach has emerged as one of the most powerful method for modeling many types of microstructure evolution processes. However, it falls short in problems where crystalline defects have a profound influence on evolution in systems. Over the last few years, the phase field crystal (PFC) method has emerged as an attractive computational approach to tackle this class of problems where atomic and continuum scales are coupled. In the PFC method the higher order gradient terms has been added to the conventional isotropic Cahn-Hilliard equation. In this approach, the decomposition produces a periodical distribution of density clusters, which is attributed to a distribution of atoms in crystals. Imperfections in this periodical distribution well mimic lattice defects, dislocations and grain boundaries, while the decomposition mimics the crystallization. Despite of a significant progress in continuum description of atomic configurations using PFC method, the physical origin of the gradient terms in this model was not established. Recently, using Atomic Density Function (ADF) theory, this problem has been resolved by Jin and Khachaturyan (JAP, 2006). It was shown that the choice of the gradient terms in PFC approach is equivalent to a smooth atom approximation. In this paper we show that the well known ADFs kinetic equations become automatically valid for the interacting atoms in the continuum when the lattice parameter of the underlying lattice is much smaller than the interaction radius, r_{int}. The relation between the ADF and Phase field approaches is under discussion.

Bootstrap percolation on complex networks

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I will present a study on bootstrap percolation on uncorrelated complex networks. I will show the phase diagram for this process with respect to two parameters: f, the fraction of vertices initially activated, and p, the fraction of undamaged vertices in the graph. Show the existence of two transitions: the giant active component appears continuously at a first threshold. There may also be a second, discontinuous, hybrid transition at a higher threshold. Avalanches of activations increase in size as this second critical point is approached, finally diverging at this threshold. Describe the existence of a special critical point at which this second transition first appears. In networks with degree distributions whose second moment diverges (but whose first moment does not), we find a qualitatively different behavior. In this case the giant active component appears for any $f > 0$ and $p > 0$, and the discontinuous transition is absent. This means that the giant active component is robust to damage, and also is very easily activated. I will also show how to formulate a generalized bootstrap process in which each vertex can have an arbitrary threshold.

The force of fluctuations

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Similar to electromagnetic vacuum fluctuations which can induce long-ranged interactions between uncharged, conducting surfaces, a rather similar effect was predicted almost 30 years ago for confined binary mixtures close to their critical point. This critical Casimir effect is due to the confinement of fluctuations in the mixture's concentration and can strongly modify the interaction potential of colloidal particles immersed in a binary fluid.

We review recent progress on the measurement of such critical Casimir forces between a colloidal particle and a flat surface in a water – 2,6-lutidine mixture. With total internal reflection microscopy (TIRM) which is capable to resolve forces down to 5 femto-Newton, we obtain distance resolved particle-wall interaction profiles. Upon approaching the critical point we observe long-ranged interactions which are attractive or repulsive depending on the specific boundary conditions of the walls. This behavior is in good agreement with recent theoretical predictions. In addition, we demonstrate, how critical Casimir forces can be used for colloidal assembly on chemically patterned surfaces.

Steering the critical Casimir effect: lateral forces, levitation, and dynamics

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The critical Casimir effect results from the confinement of the pronounced thermal fluctuations occurring upon approaching a second-order phase transition such as the demixing of a binary liquid mixture. The spatial direction of the force acting on the confining surfaces can be controlled by suitably patterning these surfaces. For a colloid close to a patterned substrate and immersed in a critical solvent a spatially confining potential can be reversibly generated, which also allows a temperature-controlled stable levitation of the particle. External perturbations affect the strength of the critical Casimir force, the time-dependence of which displays interesting features.

I will present recent results of the theoretical investigation of these various aspects, comparing them with the available experimental data.

[1] M. Troendle et al., EPL, 2009, **88**, 40004.
[2] A. Gambassi and S. Dietrich, Soft Matter, 2011, **7**, 1247.
[3] M. Troendle et al., arXiv:1012.0181.
[4] A.Gambassi, Eur. Phys. J. B, 2008, **64**, 379.

Mesoscopic theory for inhomogeneous mixtures

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Density functional theory for mixtures of spherical particles which spontaneously form inhomogeneous structures on mesoscopic length scales will be presented. Mesoscopic volume fractions will be introduced, and the grand-thermodynamic potential functional, developed in terms of them by a systematic coarse-graining procedure starting form microscopic theory, will be demonstrated. Approximate expressions for the correlation functions and for the grand potential will be discussed for weak ordering on mesoscopic length scales. Stability analysis of the disordered phase performed in mean-field approximation (MF) shows existence of either a spinodal or a λ-surface on the volume-fractions – temperature phase diagram. Separation into homogeneous phases or formation of inhomogeneous distribution of particles occurs on the low-temperature side of the former or the latter surface respectively, depending on both the interaction potentials and the size ratios between particles of different species. Beyond MF the spinodal surface is shifted, and the instability at the λ-surface is suppressed by fluctuations. We interpret the λ-surface as a borderline between homogeneous and inhomogeneous (containing clusters or other aggregates) structure of the disordered phase. Examples of interaction potentials of a simple form for one- and two-component systems will be presented in order to illustrate conditions leading to inhomogeneous structures.

A few "paradoxes" of Lévy flights

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Alpha-stable Lévy motion, also referred in physics literature as Lévy flights, stand for a class of non-Gaussian Markovian random processes whose stationary increments are distributed according to the Lévy stable probability distributions. Lévy stable laws appear as statistical description for a broad class of processes in physical, chemical, biological, geophysical, or financial contexts, among others. However, despite their popularity and numerous applications, Lévy flights are far from being well understood. I here review the properties of Lévy flights, with the particular emphasis on the first passage time and overshooting, as well as the behavior of Lévy flights in external fields, including escape from a potential well and the "Lévy ratchet". These properties are discussed on the basis of probabilistic approach, analytical and numerical solutions of space-fractional Fokker-Planck equation as well as numerical solutions of the stochastic Langevin equation with white Lévy noise.

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Oral Contributions

Abstracts

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Cooling rate dependencies across thermal phase transitions

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The state of a system taken through a phase transition is plagued with topological defects, be them domain walls, vortices, monopoles or other depending on the particular case at hand. After the quench their spatial distribution changes and, typically, their density decreases. The mechanisms whereby this occurs depend on the microscopic dynamics. Realizations of such "phase ordering kinetics" in condensed-matter are manifold including the relaxation of vortices in planar magnets or monopoles in magnetic spin-ice, both thermally quenched. The characterization of the density of topological defects has also been of interest in cosmology and the standard description in this context is given by the so-called Kibble-Zurek mechanism. We have critically revisited this theory in two characteristic cases: a second order phase transition with discrete spontaneous broken symmetry [1] and the Berezinsky-Kosterlitz-Thouless infinite order phase transition [2]. In this talk I shall explain our vision of this problem.

[1] G. Biroli, L. F. Cugliandolo, and A. Sicilia, Phys. Rev. E, 2010, **81**, 050101.
[2] A. Jelic and L. F. Cugliandolo, arXiv:1012.0417, J. Stat. Mech. (in press).

Thermodynamics of structured amorphous states: fluid, liquid, glass

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A phenomenological theoretical model of the heterophase amorphous states in the vicinity of the critical end point is developed. The model is used for description of the gas-liquid phase transformation. From one hand, the proposed model can be considered as a generalization of the Frenkel model of the heterophase fluctuations. From the other hand, it is a constructive incarnation of the Van der Waals conjecture on the decisive role of the heterophase fluctuations on the fluid state. The Widom line (continuation of the phase coexistence curve into the overcritical region) is a characteristic thermodynamic element of the model.

An analogous approach is fruitful at description of the liquid-liquid and liquid-glass continuous and discontinuous transformations. The liquid-liquid and liquid-solid heterophase amorphous states are discussed in brief.

Patchy depletion interactions

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The investigation of the entropic forces among anisotropic particles has shown that the shape of the particle can induce directionality in the depletion interaction [1]. We show how simple Asakura-Oosawa-like [2] geometrical arguments predict also a strong dependence of the depletion interaction on the local curvature of the particles. We investigate via Monte-Carlo methods the depletion interaction among a simple model of non-spherical hard particles showing how the local curvature can induce directionality in the depletion interaction. The patchy character of the resulting effective potential is a useful building brick to induce (self-)assembly [3]. Since the depletion potential depends on size and shape, and not on the chemical composition, shape-engineering of reversible depletion interactions can be applied to any particle suspension, i.e., metallic, semiconductor, or oxide [4]. We therefore believe that the ability to quantitatively predict and reversible tune the strength and the directionality of the interaction potential by solvent composition and temperature is a simple and powerful tool to control particles' assembly.

[1] E. Eisenriegler, A. Bringer, J.Phys.: Condens. Matter, 2005, **17**, S1711.
[2] S. Asakura and F. Oosawa, J. Chem. Phys., 1954, **22**, 1255.
[3] Z. Zhang, S.C. Glotzer, Nano Letters, 2004, **4**, 1407.
[4] K. Park, H. Koerner, R.A. Vaia, Nano Letters, 2010, **10**, 14331439.

Generalized excluded volume: its origin and effects

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The idea of the existence of an excluded volume (i.e., an impenetrable volume of molecules) formed the basis of the intuitive van der Waals (vdW) equation. After putting this idea on a rigorous statistical mechanical footing, the excluded volume has been used to interpret, or even estimate semi-quantitatively, a number of properties of fluids. All these facts are a consequence of the predominant effect of short- range repulsive forces acting between the molecules. This concept of the ordinary excluded volume however fails for fluids in which, in addition to omnipresent repulsive interactions at short separations, also specific short-range attractive interactions play an important role as, e.g., for associating fluids.

To model associating fluids at a very simple level, we introduced some time ago the so called primitive models which have formed later the basis of nowadays widespread SAFT method. The models mimic, by means of a square-well attraction and hard sphere repulsion, the interactions between the unlike and like interaction sites embodied to molecules, respectively, at short separations. When all attractive interactions are switched off one gets then the so called pseudo-hard body (PHB). These PHB's may be viewed as a counterpart of hard spheres and play the same role for understanding the behavior of associating fluids and developing theory thereof which hard spheres have played for simple fluids.

After a brief introduction of PHB's and their peculiar properties, a number of examples is presented showing that such generalized excluded volumes are able to explain naturally, without any parameter fitting, anomalous properties of aqueous solutions.

Worms exploring geometrical features of phase transitions

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The loop-gas approach to statistical physics provides an alternative, geometrical description of phase transitions in terms of linelike objects. The resulting statistical random-graph ensemble composed of loops and chains can be efficiently generated by Monte Carlo simulations using the so-called "worm" update algorithm. Concepts from percolation theory and the theory of self-avoiding random walks are used to derive estimators of physical observables that utilize the nature of the worm algorithm. The fractal structure of random loops and chains as well as their scaling properties encode the critical behavior of the statistical system. The general approach is illustrated for the O(1) loop model, or high-temperature series expansion of the Ising model, on a honeycomb lattice, with its known exact results as valuable benchmarks.

[1] W. Janke, T. Neuhaus, and A.M.J. Schakel, Nucl. Phys. B, 2010, **829**, 573.

Diffusion phenomena in confined liquids near the critical point

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Diffusion properties of liquid systems at reduced geometry were studied in the critical region with taking into account such three areas: 1) *fluctuation*, where singular parts of kinetic Onsager coefficients are larger than its regular parts; 2) *crossover*, where both parts of kinetic Onsager coefficients have the same order; 3) *regular*, where singular parts of kinetic Onsager coefficients are lesser than its regular parts. The influence of spatial dispersion effects and lower crossover dimensionality on diffusion properties is studied. It gives finite values of the thermo- and baroduffusion ratio and non-zeroth value of the diffusion coefficients near the critical point of bulk and confined liquids. Direct connection between the change of self-diffusion coefficient of the water molecules in the suspensions of cell's membranes and its biomedical applications are discussed.

Heterogeneous granular motors

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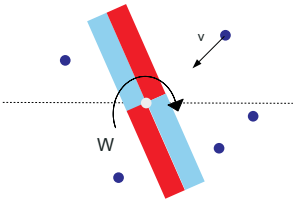

Figure 1: The chiral rotor, made with two different materials, is immersed in a bath of thermalized particles. The red and blue materials have coefficients of restitution α_+ and α_-, respectively.

Brownian ratchets, which are devices that extract work from a thermal bath, have a long history. A ratchet effect is possible whenever there is a breakdown of detailed balance and a lack of spatial symmetry [1]. The time reversal symmetry is obviously broken in collisions of inelastic particles and, as a result, several models have been proposed for granular ratchets [2–4]. Here we examine a granular chiral rotor composed of two materials with different coefficients of restitution [5]: By introducing a force-based approach [5], we calculate the mechanical power and define the efficiency of the heterogeneous rotor as the ratio of the power to the dissipation rate. An exact expression is obtained in the Brownian limit. Finally, we discuss the results in connection with recent experiments [6,7].

[1] P. Reimann, Phys. Rep., 2002, **361**, 57.
[2] G. Costantini, U.M.B. Marconi, and A. Puglisi, Phys. Rev. E, 2007, **75**, 061124.
[3] B. Cleuren, and R. Eichhorn, J. Stat. Mech., 2008, P10011.
[4] G. Costantini, U. Marini Bettolo Marconi, and A. Puglisi, Europhys. Lett., 2008, **82**, 50008.
[5] J. Talbot, A. Burdeau, and P. Viot, Phys. Rev. E, 2010, **82**, 011135.
[6] P. Eshuis et al., Phys. Rev. Lett., 2010, **104**, 248001.
[7] J. Talbot, A. Burdeau, and P. Viot, J. Stat. Mech., 2011.

A brief review on energy recycling from thermal fluctuations

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We present a brief review on some advances along the idea of recycling energy out of ambient noise by means of electro-magnetic generators as transducers. As the size of the transducers is reduced to micro and nano scales, more subtle sources of energy could be considered, for instance, Brownian motion-like or thermal fluctuations as *ambient noise*. We would like to discuss the conditions of non-equilibrium on which the second law of thermodynamics could be circumvented.

Self-propelled particles under shear

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The study of active matter has been a growing topical field of research in recent years. A suspension of self propelled (SP) particles, modeling for instance microbial or bacterial fluids, fish schools, or synthetic swimming microrobots, is a primary example of an active material. Differently from their passive counterparts, active and SP particles continuously burn energy from their surroundings or from internal sources, typically to move and this drives them out of equilibrium even in steady state. Elucidating the possibly universal properties of such active and self-propelled matter has prompted physicists to consider highly simplified models, such as the Vicsek model, which has become a paradigm in this field. This model exhibits a continuous transition from a disordered phase to an ordered one in which flocks of SP particles form and move coherently, with long range order even in 2 dimensions.

In our recent work we have extended the study of active materials to the case of externally driven, sheared, suspensions. We find that in the presence of shear (i) there is no order-disorder transition, and that (ii) coarsening of the domains is arrested so that clusters of particles assume an anisotropic shape with a well defined size decreasing with shear rate. Moreover, shear (iii) suppresses the so-called giant density fluctuations which are observed in the quiescent limit. Our results lead to a series of predictions for externally driven active systems, such as bacterial fluids, bird flocks, or even inanimate active matter such as vibrated granular rods.

Power laws and skew distributions

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Power-law distributions and other skew distributions, observed in various models and real systems, are considered. A model, describing evolving systems with increasing number of elements, is considered to study the distribution over element sizes. Stationary power-law distributions are found. Certain non-stationary skew distributions are obtained and analyzed, based on exact solutions and numerical simulations. As another example of power-law behavior, critical exponents determined from highly accurate experimental data very close to the λ-transition point in liquid helium are discussed in some detail.

In [1] some interesting ideas are developed how skew distributions such as power law, log-normal, and Weibull distributions emerge in general evolving systems and what makes the difference between them. However, we have found several problematic points in this consideration [2].

[1] Choi M.Y., Choi H., Fortin J.-Y., Choi J., Europhysics Letters (EPL), 2009, **85**, 30006.
[2] Kaupužs J., Mahnke R., Weber H., Europhysics Letters (EPL), 2010, **91**, 30004.

Critical mass and the dependency of research quality on group size

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The notion of critical mass in research is one that has been around for a long time. It has been described as some kind of threshold group size above which research standards significantly improve. However no evidence for such a threshold has been found and critical mass has never been measured - until now.

We develop a new, simple, sociophysical model which explains how research quality depends on research-group structure and in particular on size. Our model predicts that there are, in fact, two critical masses in research, the values of which are discipline dependent. Research quality is, on average, linearly dependent on group size, but only up to a limit termed the upper critical mass. Beyond this limit, a phase transition reduces the dependency of quality on quantity. The upper critical mass is interpreted as the average maximum number of colleagues with whom a given individual in a research group can meaningfully interact. Once the group exceeds this size, it tends to fragment into sub-groups and research quality no longer improves significantly with increasing size.

Our theory is tested using empirical data on the quantity and quality of scientific research groups, for which critical masses are determined. For theoretical and experimental physics, the lower critical masses are estimated to be about 6 and 13, respectively. Research groups should strive to achieve these sizes for stability. The upper critical masses, beyond which research quality does not significantly improve with group size, are about twice these values.

[1] R. Kenna and B. Berche, EPL, 2010, **90**, 58002.
[2] R. Kenna and B. Berche, Scientometrics, 2011, **86**, 527.

Critical Casimir forces for various boundary fields obtained by Monte Carlo simulation: crossover from repulsion to attraction

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The confinement of concentration fluctuations in binary liquid mixtures close to the bulk critical point generates long-ranged forces acting on the confining surfaces. In analogy with the quantum Casimir forces which are induced by vacuum fluctuations of the electromagnetic field, the forces in critical liquids are called *critical Casimir forces*. During the last two decades these phenomena have been studied experimentally, theoretically, and numerically for binary liquid mixtures (Ising model universality class) and for liquid He^4 and He^3–He^4 mixture (XY model universality class).

We have studied critical Casimir forces in 3D Ising films with surface fields by using Monte Carlo simulations. The critical Casimir force in a film of thickness L with surface fields H_1 scales as $\beta f_{\rm Cas}(T, L, H_1) = L^{-d}\theta_{\rm Cas}(L/\xi, h_1)$ where $\theta_{\rm Cas}(L/\xi, h_1)$ is a universal scaling function, ξ is the bulk correlation length, and $h_1 = H_1 L^{\Delta_1/\nu}$ is the scaling variable associated with the surface field. Here ν and Δ_1 are the correlation length and surface field critical exponents, respectively.

A numerical method based on an integration scheme for the free energy differences is used to compute the universal Casimir forces in the critical region for the Ising model for various values of the boundary fields. We study the scaling of the Casimir force as function of L/ξ and h_1 taking into account finite size corrections to scaling. We pay special attention to that region of the surface field H_1 where the force changes from repulsion to attraction upon increasing the temperature. Our results are compared with corresponding experimental data for wetting films of fluids as well as with other available theoretical results.

Nonperturbative renormalization group approach to polymerized membranes

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Polymerized membranes form a particularly rich domain of statistical physics which has known a renewed interest these last years due to the discovery of graphene, the first example of genuine two dimensional membrane. Due to their elastic properties membranes exhibit nontrivial behaviours: first, they undergo a phase transition between a crumpled phase at high temperature and a flat phase at low temperature. Second, the existence of long-range forces mediated by phonons is responsible for the stabilization of a flat phase with long-range orientational order even in dimension 2 – and less than 2 – a fact which is at the origin of the existence of, e.g., graphene-like materials. I show how a nonperturbative renormalization group approach of polymerized membranes allows to describe both qualitatively and quantitatively all these behaviours in a unified way.

Weak-universal critical behavior in the exactly solved mixed-spin Ising model with the triplet interaction on a centered square lattice

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The mixed spin-1/2 and spin-S ($S \geqslant 1$) Ising model on a centered square (union jack) lattice with the uniaxial single-ion anisotropy and the three-site three-spin (triplet) interaction is exactly solved by establishing a rigorous mapping equivalence with its corresponding symmetric (zero-field) eight-vertex model exactly solved by Baxter [1]. Within the framework of this rigorous mapping equivalence, the influence of both considered interaction parameters on the ground-state and finite-temperature phase diagrams is explored in detail. It is shown that the model under investigation exhibits a weak-universal critical behavior characterized by continuously varying critical exponents, which fundamentally depend on a relative strength of the uniaxial single-ion anisotropy and the triplet interaction. In addition, it is demonstrated that the mixed-spin Ising model with the integer-valued decorating spins S from centers of each elementary square face exhibits very different variations of the critical exponents compared to the analogous mixed-spin Ising model with the half-odd-integer spins S. The obtained rigorous results are confronted with the previously published exact results for the simple spin-1/2 Ising model with the triplet interaction on a triangular, kagomé, diced and centered square (union jack) lattice.

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[1] Baxter R.J., Exactly Solved Models in Statistical Mechanics. Academic Press, New York, 1982.

On the search for a Lifshitz point in UPd_2Si_2

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Spatially modulated systems are very common in nature. Modulated phases of various types have been observed in hundreds magnetic or ferroelectric crystals and Lifshitz points have been suggested for many of them. The phase diagrams of these systems reveal multicritical points separating the higher temperature disordered phase and the low temperature commensurate and incommensurate phases, however, the strong evidence that such a point exhibits Lifshitz type critical behavior is available only for one magnetic system, MnP. The present work on UPd_2Si_2 has been motivated by previous data on this material. The data showed that UPd_2Si_2 possesses four magnetic phases. Three ordered phases, antiferromagnetic (AFI), commensurate (LSW - Longitudinal Spin Wave structure) characterized by a propagation vector $\mathbf{Q} = (0, 0.\frac{2}{3})$, and incommensurate (ICLSW) meet at a triple point. As stated Honma et al. a probable second triple point where LSW, ICLSW, and P phases meet could not be determined by the investigation presented in their paper. The available data for the phase transition lines near this possible triple point seems to be inconsistent with LP, because the phase transition between paramagnetic and LSW phases has been suggested to be of first order. However, we have suspected that a closer study in the middle range of the magnetic field, neglected in the previous papers, might lead to the opposite conclusion. Accordingly high-quality single crystals of UPd_2Si_2 have been studied by means of heat capacity and magnetization measurements. The obtained data has yielded a $H - T$ phase diagram that significantly differs from those reported before in the literature. The main finding is identification of a multicritical point that seemingly exhibits Lifshitz characteristics. A simple phenomenological model of phase transitions near this special tricritical point is provided

Thermodynamics and dynamics of the two-state Bose-Hubbard model in the effective pseudospin representation

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Phase transition into the phase with the Bose-Einstein (BE) condensate in the Bose-Hubbard model with two local states and the particle hopping in the excited band only is investigated. Instability connected with such a transition (appearing at excitation energies δ less than the particle hopping parameter $|t_0'|$) is considered. The re-entrant behaviour of spinodales is revealed in the region of positive values of chemical potential in the hard-core boson (HCB) limit (no more than one particle per site regardless of state – excited or ground – which it occupies). Contrary to the two-level ordinary HCB case, where particles are described by the Pauli statistics, our single-site problem is a three-level one. The effective pseudospin representation is used, where operators σ_i^{α} are quite similar to spin operators for $S = 1/2$ but the anticommutator of σ_i^+ and σ_i^- is equal to the total occupation of respective states instead of unity.

It is found that the order of the phase transition can change in the case $\mu > 0$ becoming the first one. First order phase transitions also exist at negative values of δ (under the condition $\delta > \delta_{\rm crit} \approx -0.12|t_0'|$). At $\mu < 0$ the phase transition mostly remains to be of the second order. The behaviour of the BE condensate order parameter is analyzed, the (Θ, μ) and $(|t_0'|, \mu)$ phase diagrams are built and localization of tricritical points is established. A possibility of separation on the normal phase and the phase with the BE condensate at the fixed average concentration of bosons is demonstrated.

The boson Green function and the single-particle spectral density are calculated in the random phase approximation. The excitation spectrum of the "hole" type at concentrations $n \leqslant 1$ or the "particle" type at $n \geqslant 0$ has a band structure. Its reconstruction (gap disappearance and the change from the quadratic dispersion law to the linear one at $\vec{q} \sim 0$) at the first order phase transition is jump-like with a simultaneous appearance of the negative component in the spectral density.

Anharmonic effects in magnetic systems

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We describe a new mechanism leading to the formation of rational magnetization plateau phases, which is mainly due to the anharmonic spin-phonon coupling. This anharmonicity produces plateaux in the magnetization curve at unexpected values of the magnetization without explicit magnetic frustration in the Hamiltonian and without an explicit breaking of the translational symmetry. These plateau phases are accompanied by magneto-elastic deformations which are not present in the harmonic case.

Residual diamagnetism driven by the superconducting fluctuations

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The phase transition to superconducting state occurs when gauge symmetry of the system spontaneously brakes down due to appearance of the complex order parameter $\psi = \chi e^{i\phi}$. Its amplitude χ corresponds to the density of Bose-Einstein condensed fermion pairs (also indirectly manifested through energy gap at the Fermi level) whereas the phase ϕ controls coherent behavior of pairs ($\nabla\phi \neq 0$ generates supercurrents). In the case of charged particles (such as e.g. conduction band electrons) ϕ couples to the vector potential of electromagnetic field and, through the Higgs mechanism, triggers ideal diamagnetism (i.e. the Meissner effect).

We shall discuss how similar phenomena might be observable upon approaching the true phase transition T_c form above. For this purpose we explore the superconducting fluctuations between the preformed pairs (of whatever origin). Using nonperturbative method originating from the numerical renormalization group we find evidence for the residual diamagnetic response and remnants of the sound-wave Goldstone mode above T_c. We confront our study with the recent experimental data obtained for cuprate superconductors and other correlated fermion systems.

Dynamics in disordered media: Applications to biophysics, mathematical finance and etc.

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In this talk we overview some known and novel results on different characteristics of diffusion in random environments, such as, e.g., mean-square displacements, currents, hitting probabilities. We will discuss, as well, the relation of these characteristics to the kinetics of helix-coil transitions in heteropolymers, Black-Scholes model of stock options evolution and some statistics of partial and proper delay times of Wigner-Smith time delay matrices.

Subdiffusion with a time-dependent force: the case of under- and overshooting subordination

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In this report we extend borders in the analysis of anomalous diffusion with an arbitrary space-time-dependent driving. Our method is based on the Langevin-type dynamics with subordination technique in which there is a coupling between the α-stable Lévy process and its inverse as applied to the description of fractional subdiffusion. This leads to two different compound subordinators. One of them underestimates the real time t, and another overestimates it. The stochastic processes are quiet different. The first has all finite moments, and the second has no any finite moment. In both cases by direct calculations we establish the two significant physical properties – "death of linear response" (the mean particle position stagnates) and "field-induced dispersion" (asymptotic growth of the field-dependent second moment) typical for the subdiffusion with a harmonic time-dependent potential. These effects are described by well-known special functions.

The critical behavior of Hamiltonian type in driven and coupled dissipative systems

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The period-doubling transition to chaos in dissipative system demonstrates scaling properties with definite scaling factors revealed by M. Feigenbaum [1] using the renormalization group. In Hamiltonian systems period-doubling transition also occur but with another scaling factor, so corresponding type of critical behavior is usually referred as Hamiltonian, or H-type[2, 3].

In this presentation we show that this critical behavior is rather typical for dissipative dynamical systems as the codimension two phenomenon.

First we investigate the evolution of the Feigenbaum critical line in the system of two coupled Hénon maps [4] while the dissipation decreases. We show that gaps occur on the Feigenbaum critical line when the dissipation becomes rather small (but definitely non-zero so the system remains dissipative). We reveal the bifurcation scenario of those transformations and show that Feigenbaum critical line terminates at the critical points of H and C types after the gaps occur.

Another system under investigation was the Van-der-Pole oscillator driven by nonlinear pulses. We show that the H critical point as the codimension two phenomenon ca be observed by adjusting the pulses amplitude and the dissipation of the oscillator.

[1] Feigenbaum M.J., J. Stat. Phys., 1978, **19**, No. 1, 25.
[2] MacKay R.S. – In: Long Time Predictions in Dynamics. J. Wiley and Sons, New York, 1983.
[3] Kuznetsov A.P., Kuznetsov S.P., Sataev I.R., Physica D, 1997, **109**, 91.
[4] Hénon M., Comm. Math. Phys., 1976, **50**, 69.

Efficient quantum information transfer through a uniform channel

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Effective quantum-state and entanglement transfer can be obtained by inducing a coherent dynamics in quantum wires with homogeneous intrawire interactions. This goal is accomplished by optimally tuning the coupling between the wire endpoints and the two qubits there attached. A general procedure to determine such value is devised, and scaling laws between the optimal coupling and the length of the wire are found. The procedure is implemented in the case of a wire consisting of a spin-$\frac{1}{2}$ XY chain: results for the time dependence of the quantities which characterize quantum-state and entanglement transfer are found of extremely good quality also for very long wires. The present approach does not require engineered intrawire interactions nor a specific initial pulse shaping, and can be applied to a vast class of quantum channels.

[1] Banchi L., Apollaro T.J.G., Cuccoli A., Vaia R., Verrucchi P., Phys. Rev. A, 2010, **82**, 052321.

Manipulating and protecting entanglement by means of spin environments

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We study the dynamical behavior of two initially entangled qubits, each locally coupled to an environment embodied by an interacting spin chain. We consider energy-exchange qubit environment couplings resulting in a rich and highly non trivial entanglement dynamics. We obtain exact results for the time-evolution of the concurrence between the two qubits and find that, by tuning the interaction parameters, one can freeze the dynamics of entanglement, therefore inhibiting its relaxation into the spin environments, as well as activate a sudden-death phenomenon. We also discuss the effects of an environmental quantum phase transition on the features of the two-qubit entanglement dynamics.

[1] Apollaro T.J.G., Cuccoli A., Di Franco C., Paternostro M., Plastina F., Verrucchi P., New J. Phys., 2010, **12**, 083046.

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Posters

Abstracts

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Piezoelectric resonance in Rochelle salt

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A dynamic dielectric response of Rochelle salt is studied within the framework of the two-sublattice Mitsui model completed by piezoelectric interaction of the pseudospin system with the shear strain ε_4. Interaction with transverse field, attributed to ordering units flipping between two equilibrium positions, is taken into account. Special attention is given to the research of dynamic dielectric permittivity of free crystal. Developed approach explains the piezoelectric resonance phenomena and corrects some flaws of previous work [1]. It is shown, the equations describing piezoelectric resonance in the vicinity of transition point and the same equations distant from the transition point are different.

[1] A.P. Moina, R.R. Levitskii, and I.R. Zachek, Phys. Rev. B, 2005, **71**, 134108.

Phase diagrams of spin-3/2 Blume-Capel model on rectangular lattice under longitudinal magnetic field

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The spin-3/2 Blume-Capel model on a rectangular lattice

$$H = -\sum_{i=1}^{L}\sum_{j=1}^{L}\Big[\Gamma^z S^z_{i,j} + D(S^z_{i,j})^2 + K^F S^z_{i,j}S^z_{i+1,j} + K^A S^z_{i,j}S^z_{i,j+1}\Big]$$

with the ferromagnetic bilinear short-range interaction ($K^F = 1+x$, $x \in [-1,1]$) in one direction and the anti-ferromagnetic one ($K^A = -1+x$) in the perpendicular direction under a longitudinal magnetic field Γ^z and in the presence of a single-ion anisotropy D is investigated within the mean field approximation. The phase diagrams in the (x, temperature) plane are constructed for different values of the longitudinal magnetic field and the single-ion anisotropy.

Non-Markov kinetic equation for quantum plasma with exchange interaction

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In the quantum kinetic equation for weakly coupled polarizable plasmas which was derived by Balescu, and Guernsey [1, 2] the exchange interaction of particles was retained only in the distribution functions. But it is also necessary to consider the exchange interaction in the scattering amplitude and in the dielectric function. Moreover, the Balescu equation involves the polarization of the system only in the collision integral, while the thermodynamics corresponds to the ideal gas; the dissipative and non-dissipative phenomena are not treated on the equal footing. This discrepancy can be avoided if non-Markov effects are considered [3]. Starting from the quantum BBGKY-hierarchy for the statistical operators, we have solved, in the so-called plasma approximation, the equation for the quantum pair correlation function the non-Markov correction being included. The solution of this equation can be expressed in terms of the resolvent of the linear Hartree-Fock equation. As a result, we obtain a quantum non-Markov kinetic equation, which involves both the dynamical screening of the interaction potential and the exchange interaction in a non-trivial way [4]. In particular, this equation contains the dielectric function which exactly describes the exchange scattering in plasma. The quantum kinetic equation derived satisfies the low of total conservation with regard for the polarization and the exchange interaction. The similar result was found for electric field fluctuations in the systems of the charged particles with exchange interaction [5].

[1] Balescu R., Phys. Fluids, 1961, **4**, 94.
[2] Guernsey R.L., Phys. Rev., 1962, **127**, 1446.
[3] Belyi V.V., Kukharenko Yu.A., Wallenborn J., Phys. Rev. Lett., 1996, **76**, 3554.
[4] Belyi V.V., Kukharenko Yu.A., J. Stat. Mech., 2009, P06002.
[5] Belyi V.V., Kukharenko Yu.A., Contrib. Plasma Phys., 2009, **49**, 550.

Shape anisotropy of polymers in porous environment

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We study the influence of structural obstacles in a disordered environment on the size and shape characteristics of long flexible polymer macromolecules. We use the model of self-avoiding random walks on diluted regular lattices at the percolation threshold in space dimensions $d = 2$, 3. Applying the Pruned-Enriched Rosenbluth Method (PERM), we numerically estimate rotationally invariant universal quantities such as the averaged asphericity A_d and prolateness S of polymer chain configurations. Our results quantitatively reveal the extent of anisotropy of macromolecules due to the presence of structural defects.

Noise and retardation effects in the Landau-Lifshitz-Gilbert equation

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The Landau-Lifshitz-Gilbert equation describing the precession and the damping of collective spin wave excitations is generalized twofold, by the inclusion of retardation effects as well as stochastic magnetic fields. In case of a pure spatial dependent retardation kernel of the width ξ and the strength Γ_0, the self-organized internal magnetic field is supplemented by a time dependent stochastic force of strength D and a finite correlation time τ_c. The corresponding Fokker-Planck equation enables us to calculate the mean values of the components of the magnetization. Within the spin wave approximation, valid in the long wave-length limit, we find an analytical solution for the dispersion relation and the damping of the spin wave excitation. In particular, we analyze the spin-wave life-time τ_L and the line width ΔB according to ferromagnetic resonance (FMR) experiments in dependence on the before introduced quantities. Whereas the life-time decreases with increasing temporal noise strength D, retardation strength Γ_0 as well as correlation time τ_c it is enhanced for growing width ξ of the spatial kernel. In the same manner we calculate the measurable FMR-line width ΔB depending on the model parameters, e.g. it offers a strong increase when the correlation time τ_c ranges in the nanosecond interval.

Spin and charge correlations in quantum dots: an exact solution

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The inclusion of charging and spin-exchange interactions within the Universal Hamiltonian description of quantum dots is a highly non-trivial problem owing to the fact that it leads to a formulation of the problem in terms of a non-Abelian action. We present an exact analytical solution of the problem, in particular, in the vicinity of the Stoner instability point. We calculate several physical observables, including the tunneling density of states (TDOS) and the spin susceptibility [1]. Due to the presence of spin-exchange interaction, at the vicinity of the instability point the TDOS exhibits a non-monotonous behavior as function of the tunneling energy. This effect survives even at temperatures higher than the exchange energy. Our results for the spin susceptibility and TDOS are extended to the presence of the Zeeman splitting [2]. Our approach is generalizable to a broad set of observables, including the a.c. susceptibility and the absorption spectrum for anisotropic spin interaction. Experimentally, our results could be tested in nearly ferromagnetic materials. This analysis is a first step towards solving more complicated problems of transport in quantum dots with spin-exchange interaction, addressing such effects as level statistics at low temperatures, superconducting fluctuations, and non-equilibrium conditions.

[1] Burmistrov I.S., Gefen Yu., Kiselev M.N., JETP Lett., 2010, **92**, 179.
[2] Burmistrov I.S., Gefen Yu., Kiselev M.N., Medvedovsky L., in preparation.

Bistability and oscillatory behavior in heterogeneous catalysis: CO oxidation reaction

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CO_2 formation through catalytic oxidation of CO is one of the prototypical surface reactions that has been extensively studied in recent years [1]. Much of today's insight in heterogeneous catalysis arises from this model system. The scientific interest in the study of these processes is due to emergence of a rich and complex variety of physical-chemistry phenomena including chaotic behavior, bistability, critical phenomena and phase transitions, oscillatory behavior and so on.

The goal of this work is to investigate a kinetic model for the catalytic CO oxidation on a Pt(110) surface at low pressures and to find the conditions at which the bistability and oscillatory behavior appears. We have established that, at intermediate pressures, two stable states exist, and the system exhibits jumps from one stable branch onto the other. This is the bistability phenomenon. The condition of existence of the bistable region for the model has been analytically found, and the bifurcation diagram has been constructed.

From the analysis of stability phase diagram of the model in the $(p_{\mathrm{CO}}, p_{\mathrm{O}_2})$ parameter plane has been constructed. We have found two types of the stationary points which present two different stability regimes, namely the stable and the unstable oscillatory ones. Oscillatory regime arises because of the interplay between bistability and adsorbate-induced surface reconstruction $1 \times 2 - 1 \times 1$ exposing patches with different O_2 sticking probabilities [2].

[1] Yu. Suchorski, Ch. Spiel, D. Vogel, W. Drachsel, R. Schlogl, and G. Rupprechter, Chem. Phys. Chem., 2010, **11**, 3231.
[2] I.S. Bzovska and I.M. Mryglod, Condens. Matter Phys., 2010, **13**, 34801.

The kinetics of the order-disorder transition in the models of dynamic synchronization

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In this report we consider the kinetic of order-disorder transition in two basic models of the dynamical synchronization. They are the Vicsek model (VM) for the self-propelled particles and the Kuramoto model (KM) for the coupled oscillators. The kinetic of both models are studied within the Langevin equation:

$$\mathrm{d}\theta = Kr\sin\theta\mathrm{d}t + b(\theta,\eta,r)\mathrm{d}w$$

where θ_i is the pase angle of i-th particle, $r = 1/N\sum_j \mathrm{e}^{\mathrm{i}\theta_j}$ is the order parameter, K is the interaction strength . The correlation between the order parameter and the spatial particle density is neglected.

In VM K is the average number of nearest neighbors in the case that they this number has a Poisson distribution. In the KM it is just the strength of interaction between oscillators.

For the corresponding Fokker-Planck equation the stationary distribution function is found. The self-consistent equation for the order parameter is obtained and solved for different types of noises: the scalar noise ($b(\theta,\eta,r) = \mathrm{const} = b_s$), the vector noise ($b(\theta,\eta,r) = b_v(\theta,\eta,r)$), and the mixed noise ($b_{\mathrm{mix}}(\theta,\eta,r) = b(b_{\mathrm{s}}, b_{\mathrm{v}})$). The dependence of the type of order-disorder transition on the properties of function $b(\theta,\eta,r)$ is demonstrated. The phase diagram of mixed noise is obtained and the existence of tricritical point is predicted.

The kinetic approach is proposed that will take into account the correlations between the velocity and density fields. This is needed to build a hydrodynamic description of such system. The vortices that appear in the VM simulation are studied numerically. It is shown that the relaxation time of a vortex is proportional to the noise strength and decreases as the number of nearest neighbors is increased. This results agree qualitatively with the theoretical results of the hydrodynamic model of [Kulinskii et al., Europhys. Lett., 2005, **71**, 207].

Exactly solvable random spin-$\frac{1}{2}$ XX chain with three-site interactions

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We consider the spin-$\frac{1}{2}$ XX chain with three-site interactions in a random (Lorentzian) transverse field. The Hamiltonian of the model reads [1]

$$\begin{aligned} H &= \sum_n \big[J \left(s_n^x s_{n+1}^x + s_n^y s_{n+1}^y \right) \\ &\quad + K \left(s_n^x s_{n+1}^z s_{n+2}^x + s_n^y s_{n+1}^z s_{n+2}^y \right) + \Omega_n s_n^z \big] . \end{aligned}$$

Here J and K are the interaction constants and Ω_n is the external transverse magnetic field on the site n. The on-site fields are assumed to be independent random variables each with the Lorentzian probability distribution $p(\Omega_n) = (1/\pi)\{\Gamma/[(\Omega_n - \Omega_0)^2 + \Gamma^2]\}$. The introduced spin model can be mapped via the Jordan-Wigner transformation onto a tight-binding model of spinless fermions with nearest and next-nearest hopping and random on-site energy. Furthermore, exploiting the old Lloyd's idea [2], the random-averaged Green functions can be obtained. As a result, we obtain exact analytical results for the random-averaged density of states and thermodynamic quantities.

The nonrandom counterpart of the spin model has a rich ground-state phase diagram exhibiting quantum phase transitions. With our results for the thermodynamic quantities we discuss how the quantum critical behavior is modified by randomness.

For further details see Refs. [1].

[1] Derzhko V., Derzhko O., Richter J. Preprint arXiv:1012.2058.
[2] Lloyd P., J. Phys. C, 1969, **2**, 1717.

Statistical mechanics of Rotating Gas

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Statistical mechanics for an ideal gas that is in equilibrium with rotating cylindrical envelope is formulated. An average angular velocity of the gas is introduced. The equilibrium conditions are the equalities of the temperature and the angular velocity of the gas and the envelope. The free energy of gas is obtained in classical mechanics from the Gibbs distribution. The thermodynamical potential for the non-degenerate gas is computed in quantum mechanics. They are functions of the temperature, the angular velocity, the height and the sectional area of cylinder.

Exact results of the mixed spin-1/2 and spin-1 Ising model on a decorated Bethe lattice

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The mixed spin-1/2 and spin-1 Ising model on a decorated Bethe lattice with the general coordination number q is exactly solved by using the decoration-iteration mapping transformation with the rigorous method based on exact recursion relations. The exact solution is obtained by mapping the mixed spin-1/2 and spin-1 Ising model onto the spin-1/2 Ising model on the Bethe lattice. In particular, the effect of the uniaxial single-ion anisotropy on the magnetic properties (phase transitions, sublattice and total magnetizations, compensation temperatures) are investigated. It is shown that the finite-temperature phase boundary lines between the ordered and disordered phases basically depend on the coordination number q of the Bethe lattice and exchange parameters in the model Hamiltonian. The possibility of reentrant regions in phase diagrams have been also studied for different coordination number of lattice. For the zero value of exchange parameter between the spin-1/2 atoms in the Hamiltonian, the critical lines approach to the zero-temperature phase boundary at D/J with a negative (positive) slope for the Bethe lattice with the coordination number $q < 4$ ($q > 4$) and with an infinite gradient for the particular case with coordination number, $q = 4$. We also show that the model can exhibit two compensation temperatures when the decorating spin is $S = 1$.

Non-identity in system of coupled elements

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Investigators give recently much attention to the investigation of complex systems and networks. It is very difficult and sometimes impossible to obtain analytical solutions of the equations describing such systems. Computer simulation helps to solve this problem. But investigators have generally restricted themselves to the assumption that coupled systems are identical (with identical parameters), because this assumption allows to simplify obtained equations and their solutions. At the same time it is practically impossible to obtain complete identity of coupled systems or elements of the network.

It is shown in this work that non-identity in parameters of coupled systems results in essentially new effects and regimes of their behavior, and these effects become apparent not only in systems with large quantity of coupled elements, but even if there is only two coupled elements. One of such effects is the "broadband synchronization". There are presented in this work the results of numerical and experimental research of the basic model in nonlinear theory demonstrating the phenomenon of mutual synchronization. Namely, it is the system of two coupled van der Pol oscillators with non-identical controlling parameters. There are presented also the results of investigation of interaction between self-oscillating different nature elements, namely, Kislov-Dmitriev generator and van der Pol oscillator, brusselator and van der Pol oscillator.

Static quadrupolar susceptibility for the Blume-Emery-Griffiths Model

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Response of dipolar order parameter or magnetization (M) to the external magnetic field (H) is called dipolar (or magnetic) susceptibility (χ_M). Similarly, a linear response of the quadrupolar order parameter (Q) to the crystal field (Δ) which is linearly coupled to the quadrupolar field in the Blume-Emery-Griffiths (BEG) model can be interprated as the quadrupolar susceptibility (χ_Q). In this study, we have made use of mean-field (MF) self-consistent equations for the BEG model to derive static expressions for both χ_M and χ_Q. Temperature behaviours of both susceptibilities near the phase transition point have been analyzed. It is found that while MF expression for χ_M has a divergence at the critical temperature (T_C), χ_Q displays a jump-discontinuity behaviour at the transition temperature T_C .

Structures on lattices: Some useful relations

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In many methods for the determination of the ground states of lattice-gas models (or equivalent spin models) the global ground-state structures are constructed with local configurations of some subset of the lattice (cluster). We show that there exist some linear relations between fractional contents of these configurations in any structure that they generate.

Consider cluster $\mathbf{K}$, which covers the lattice with overlaps and a set of its configurations $\{\mathbf{K}_l\}$ $(l = 1, 2, ..., L)$. Consider subcluster $\mathbf{Q}$ of this cluster. Let the subcluster occupy M *nonequivalent* positions in the cluster $(m = 1, 2, ..., M)$. Let each cluster $\mathbf{Q}$ on the lattice be contained in c_m clusters $\mathbf{K}$ as subcluster $\mathbf{Q}$ in position number m. Consider a structure $\mathbf{S}$ on the lattice generated by the set of cluster configurations $\{\mathbf{K}_l\}$. This means that each cluster $\mathbf{K}$ on the lattice has one of the configurations of the set. We denote the fractional content of configuration $\mathbf{K}_l$ in structure $\mathbf{S}$ by k_l $(\sum_l k_l = 1)$.

Consider a subcluster configuration $\mathbf{Q}_t$ from the set of all possible subcluster configurations $\{\mathbf{Q}_t\}$ and calculate its content in structure $\mathbf{S}$. This can be done in different ways, depending on the position of the subcluster in the cluster. Let it be position m. Then the number of configurations $\mathbf{Q}_t$ per one cluster $\mathbf{K}$ is equal to $\sum_l \frac{k_l n_{ml}}{c_m}$, where n_{ml} is the number of configurations $\mathbf{Q}_t$ occupying position m in configuration $\mathbf{K}_l$ of the cluster. The number of configurations $\mathbf{Q}_t$ should not depend on m. Therefore the following relation holds: $\sum_l \frac{k_l n_{m_1 l}}{c_{m_1}} = \sum_l \frac{k_l n_{m_2 l}}{c_{m_2}}$, where m_1 and m_2 are arbitrary *nonequivalent* positions of subcluster $\mathbf{Q}$ in cluster $\mathbf{K}$. This equality gives a relation between fractional contents k_l. Considering different pairs of positions of the subcluster in the cluster or another subclusters, we obtain other relations. Such relations can be useful for the determination of the ground states of lattice-gas models.

[1] Yu.I. Dublenych, Phys. Rev. E, 2011, **83**, 022101.

Localization transition in binary mixture with high mass asymmetry

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We consider a mixture of interacting particles with two different masses (m_1 and m_2) but otherwise equal proerties (e.g. size, interaction strength) at different number densities and concentrations. For the transport coefficients like mass diffusion and viscosity at lower densities a Stokes relation holds over a large range of concentrations x of the heavy particles [1]. Here we report simulations at higher densities and compute the mass diffusion coefficient for both types of particles at different concentrations x and mass ratios $\mu = m_2/m_1$. Increasing the mass ratio one expect to reach in the limit of $\mu \to \infty$ the model of a liquid in a fixed random matrix with finite diffusion coefficent D_1 for the light particles. However at higher density we observe a localization transition at a concentration dependent high but finite value for the mass ratio. At the transition both mass diffusion coefficents go to zero. Moreover in the region where such a transition exists the values of D_1 and μD_2 seem to become equal. Near the transition at μ_c the mass diffusion coefficients decrease to zero with a power law $D_i \sim (\mu_c - \mu)^z$ and an exponent z of about 2.1.

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[1] W. Fenz, M. Mryglod, O. Prytula, and R. Folk, Phys. Rev. E, 2009, **80**, 021202.

A new technique for complete enumeration of self-avoiding walks (SAWs) on percolation clusters

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The critical behavior of SAWs on disordered lattices has been studied extensively in recent decades. Of particular interest is the situation at the percolation threshold where the fractal dimension changes. Unfortunately, the strong disorder poses a problem for Monte Carlo methods. Straightforward enumeration, on the other hand, may benefit from the reduced number of conformations at criticality but still suffers from exponential increase in computation time with the length of the walk.
Here, a more effective enumeration scheme is presented. Exploiting the structural properties of the critical percolation cluster, it essentially removes the exponential increase in complexity. This permits studying walks of several hundred steps (involving effective enumeration of more than 10^{30} chains).

On quantum kinetic evolution of marginal observables

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We develop a rigorous formalism for the description of the evolution of observables of quantum systems of particles in the mean-field scaling limit. The corresponding asymptotics of a solution of the initial-value problem of the dual quantum BBGKY hierarchy is constructed. Moreover, links of the evolution of marginal observables and the evolution of quantum states described in terms of a one-particle marginal density operator are established. Such approach gives the alternative description of the kinetic evolution of quantum many-particle systems to generally accepted approach on basis of kinetic equations.

[1] Gerasimenko V.I., Ukr. Phys. J., 2009, **54**, No. 8–9, 834–846.
[2] Borgioli G., Gerasimenko V.I., Nuovo Cimento C, 2010, **33**, No. 1, 71–78.
[3] Gerasimenko V.I., Kinetic and Related Models, 2011, **4**, No. 1 (submitted for publication).

A molecular dynamics study of collective dynamics in a binary glass

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Collective dynamics and acoustic excitations in disordered solids are of great interest because of many unusual features. In particular an issue of the origin of so-called boson peak is still unsolved, although there were many attempts to explain it. In this study we tried to shed light on the problem of collective excitations in binary glasses and boson peak in particular.

Extensive molecular dynamics simulations were carried out for the binary Lennard-Jones mixture within the Wahnström model [1]. We calculated total and concentration dynamic structure factors and corresponding current spectral functions. From their peak position we were able to obtain dispersion curves of longitudinal and transverse collective excitations. We have also applied the novel approach by Shintani and Tanaka [2] that made possible the formal consideration of transverse analogy of dynamic structure factors. We have found, that concentration dynamic structure factors in contrast to total dynamic structure factors contain pronounced low-frequency peaks that presumably are responsible for the boson peak formation in the binary glass. The motion of individual atoms in the mixture was analyzed with the purpose to connect its features fo the low-frequency modes responsible for boson peak.

[1] T. Schrøder, S. Stastry, J. Dyre and S. Glotzer, J. Chem. Phys., 2000, **112**, 9834.
[2] H. Shintani and H. Tanaka, Nature Mater., 2008, **7**, 870.

Impact of asymmetry on phase transitions in the presence of an intermediate metastable state

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It was discovered in supercooled liquids of o-benzylphenol [1], salol (phenyl salicylate) and 2,2'-dihydroxybenzophenone that crystal nuclei are generated and extinguished after the liquids have been cooled rapidly below the glass transition temperature. Stochastic generation and extinction of crystal nuclei may be described as a result of fluctuation of the cluster structure of non-equilibrium supercooled liquid. Another liquid phase with a structure different from the ordinary one could be generated in a similar procedure, and a liquid-liquid phase transition found experimentally in real systems is closely related to this phenomenon.

A Landau-type potential-based kinetic model involving one order parameter has been developed to study the impact of both asymmetry and external field on phase transitions in the presence of an intermediate metastable state [2], thus allowing looking, in particular, into the heterogeneous structure relaxation in such materials. Depending on the values of its control parameters, the potential has one, two or three possible minima, and we study the problem by construction of the equilibrium phase diagrams. The analytical solutions of the problem were investigated, and the model provides a set of three control parameters necessary to realize different transition scenarios in each case, which therefore assign to this model a high degree of universality as long as the respective control parameters are suitably varied. We found that the role of cubic term in order parameter of the Landau-type potential associated to the asymmetry of the system is to increase the stability of new phase for the suitably varied control parameter. In particular, our results support the 'cluster structure model' of supercooled liquids and glasses, according to which the role of heterogeneity in nucleation is to enhance the generation of crystal nuclei as clusters of the new phase.

[1] Paladi F., Oguni M., Phys. Rev. B, 2002, **65**, 144202.
[2] Paladi F., Physica A, 2010, **389**, 1986.

Conformational transitions in semiflexible polymers

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We study the conformational properties of semiflexible polymers within the lattice model of self-avoiding random walks (SAW) with bending energy ε dependence on orientation between successive steps [1]. We apply the pruned-enriched Rosenbluth method (PERM) [2]. Both the cases of bending preference ($\varepsilon < 0$) and unfavorableness ($\varepsilon > 0$) are analyzed, and details of "coil-to-rod" transition as well as transition into the "superflexible" state are discussed. The existence of marginal value of $\varepsilon \simeq -3.5$ is obtained, below which the polymer chain consisting of N monomers, has $N - 1$ bendings and thus is in a "superflexible" state.

[1] J.W. Halley, H. Nakanishi, R. Sandararajan, Psys. Rev. B, 1985, **31**, 293.
[2] P. Grassberger, Phys. Rev. E, 1997, **56**, 3682.

Modelling speciation in nitric acid solutions using the Associative Mean Spherical Approximation

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A model is developed to describe the thermodynamic properties (osmotic and activity coefficients) and the degree of association of associating electrolytes. It is assumed that the cation and the anion can form two different kinds of pair: a solvent separated ion pair and a chemical pair (undissociated molecule). The model is an extension of the associative (binding) mean spherical approximation (AMSA or BiMSA), in which the size and charge of the ions in the chemical pair may differ from those of the free ions. Corrections arising from the description of the chemical equilibria conditions at Lewis-Randall (constants pressure) state, instead of McMillan-Mayer (constant solvent chemical potential) state, are taken into account in the model. The model is then applied to solutions of nitric acid for which experiment suggests the formation of two ion pairs. A fit of the osmotic coefficient and the proportion of free ions (obtained from Raman spectroscopy experiments), leads to a determination of the speciation in nitric acid solutions.

Exploration of a radial bus system: Modelling and optimisation

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This work explores possibilities for finding optimal geometries for a bus system servicing an extended area with constant density of population that is dedicated to offer transport from any point of this area to the center. Optimization is an important issue, in particular for public transport networks. There is quite number of works published in this field, however these are mostly concerned with traffic jams, schedules, logistics, etc. Here we study another interesting question. Given a city that extends over a circular area with an overall constant population, can the topology of the public transport network (including trams, buses and other kinds of public transport operating in the city) be optimized and in what way. That is quite different from the usual problem of optimizing transport between a set of given sites leading to a combinatorial problem [1-3]. We will be looking at simple topologies, having more or less only one input parameter - the number of buses Nb running on this network. This number is essentially determined by the amount the city is willing to invest. The aim is to optimize either the average travelling time of all citizens, or their mean velocity, while travelling.

[1] S.B. Pattnaik et al., JTE, 1998, **368**.
[2] D.L. Van Oudheusden et al., Transportation, 1987, **14**.
[3] G.F. Newell, Transportation Science, 1979, **13**.

Aspect-ratio dependence of thermodynamic Casimir forces

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We consider three-dimensional Ising models in a $L_\perp \times L_\parallel \times L_\parallel$ cuboid geometry with finite aspect ratio $\rho = L_\perp/L_\parallel$ and periodic boundary conditions along all directions [1]. For these models the universal finite-size scaling function of the thermodynamic Casimir force in $\perp$ direction is evaluated numerically by means of Monte Carlo simulations employing the method recently presented in [2]. The Monte Carlo results are compared to recent field theoretical results for the Ising universality class for temperatures below and above the bulk critical temperature T_c [3], and to the finite-size scaling functions of the thermodynamic Casimir force derived in [4] for the $O(n)$-symmetrical case and temperatures $T \geq T_\mathrm{c}$ in the framework of the renormalization group-improved perturbation theory to two-loop order. The MC data are found to be in good agreement with these field theoretical results. Furthermore, the Casimir force scaling function for the two dimensional Ising model as function of ρ is calculated exactly and compared to the three dimensional case. We give a general argument that the Casimir force at the critical point vanishes for $\rho = 1$ and becomes positive for $\rho > 1$.

[1] A. Hucht, D. Grüneberg and F. Schmidt, arXiv:1012.4399, 2010.
[2] A. Hucht, Phys. Rev. Lett., 2007, **99**, 185301.
[3] V. Dohm, Europhys. Lett., 2009, **86**, 20001.
[4] D. Grüneberg and H. W. Diehl, Phys. Rev. B, 2008, **77**, 115409.

Transport coefficients of a dense fluid mixture with multistep interaction between particles

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Using the kinetic theory for systems with multistep interaction between particles, we obtain analytical expressions for transport coefficients of a dense fluid mixture. The collision integral of the theory takes explicitly into account pair processes between particles occurring at separations of interparticle attraction. The kinetic equation for the one-particle distribution function is complemented by the potential energy density equation. As a closure relation for the pair distribution function, we adopt the approximation of nonuniform equilibrium proposed for hard spheres [1] and square-well particles [2]. It is formulated in terms of the number density fields and the inverse potential quasi-temperature, an additional non-equilibrium parameter.

We consider contributions of the first order in gradients to the stress tensor, heat flux, and diffusion flux of mass and find out expressions for the linear transport coefficients.

Special attention is payed to the terms caused by the non-equilibrium correction to the pair distribution function, which manifest themselves in the coefficients of bulk viscosity and thermal conductivity.

The results are compared with those of previous works [3–6].

[1] H. van Beijeren, M.H. Ernst, Physica (Utrecht), 1973, **68**, 437.
[2] J. Karkheck et al. Phys. Rev. A, 1985, **32**, 2517.
[3] H.T. Davis et al., J. Chem. Phys., 1961, **35**, 2210.
[4] H. van Beijeren, J. Karkheck, J.V. Sengers, Phys. Rev. A, 1988, **37**, 2247.
[5] M.V. Tokarchuk, I.P. Omelyan, Ukr. J. Phys., 1990, **35**, 1255.
[6] M.V. Tokarchuk, I.P. Omelyan, A.E. Kobryn, Phys. Rev. E, 2000, **62**, 8021.

Coherence, decoherence, and memory effects in the problems of quantum surface diffusion

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We consider surface diffusion of a single particle, which performs site-to-site under-barrier hopping, fulfils intrasite motion between the ground and the first excited states within a quantum well, and interacts with surface phonons. On the basis of quantum kinetic equations for one-particle distribution functions [1] we study the coherent and incoherent motion of the adparticle. In the latter case we derive the generalized diffusion coefficients and study various dynamic regimes of the adparticle [2]. The critical values of the coupling constant $G_{cr}(T, \Omega)$, which separate domains with possible recrossing from those with the monotonic motion of the adparticle, are calculated as functions of a temperature T and a vibrational frequency Ω. These domains are found to coincide with the regions where the experimentally observed diffusion coefficients change their behavior from weakly dependent on T to quite a sensitive function of the temperature. We also evaluate the off-diagonal (relative to the site labels) distribution functions both in the Markovian limit and when the memory effects become important. The obtained results are considered in the context of the "long tails" problem of the generalized diffusion coefficients, the recrossing/multiple crossing phenomena, possible appearance of the frustrated translational mode (T-mode) of the adsorbate, and an eventual interrelation between the adparticle dynamics at short times and the temperature dependence of the diffusion coefficients measured experimentally.

[1] V.V. Ignatyuk, Phys. Rev. E, 2009, **80**, 041133.
[2] V.V. Ignatyuk, Preprint: Cond-mat.stat-mech/1012.1491v1.

Computer simulation of a self-assembly of liquid crystalline dendrimers

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A coarse-grained simulation model for a third generation liquid crystalline dendrimer is presented. It allows, for the first time, for a successful molecular simulation study of a relation between the shape of a polyphilic macromolecular mesogen and the symmetry of a macroscopic phase. The model dendrimer consists of a soft central sphere and 32 grafted chains each terminated by a mesogen group. The mesogenic pair interactions are modelled by the soft core spherocylinder model of Lintuvuori and Wilson.

Coarse-grained molecular dynamics simulations are performed on a melt of 100 molecules in the anisotropic-isobaric ensemble. The model of liquid crystalline dendrimer shows conformational bistability, with both rod-like and disc-like conformations stable at lower temperatures. Each conformation can be induced by an external aligning field of appropriate symmetry that acts on the mesogens (uniaxial for rod-like and planar for disc-like), leading to their self-assembly into a monodomain smectic A or a columnar phase, respectively. Both phases are stable for approximately the same temperature range and both exhibit a sharp transition to an isotropic cubic-like phase upon heating. We observe a very strong coupling between the conformation of the macromolecule and the symmetry of a bulk phase, as suggested previously by theory.

[1] I.M. Saez and J.W. Goodby, Liquid Crystalline Functional Assemblies and Their Supramolecular Structures, 2008, **128**, 1.
[2] M.R. Wilson, J.M. Ilnytskyi and L.M. Stimson, J. Chem. Phys., 2003, **119**, 3509.
[3] J.S. Lintuvuori and M.R. Wilson, Phys. Chem. Chem. Phys., 2008, **128**, 044906.
[4] J.M. Ilnytskyi, J.S. Lintuvuori and M.R. Wilson, Condens. Matt. Phys., 2010, **13**, 33001.

Magneto-sensitive elastomers in a homogeneous magnetic field: a regular rectangular lattice model

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A theory that describes mechanical properties of the magneto-sensitive elastomers is developed in the framework of a linear elasticity approach. A model is used in which magnetic particles are located on the sites of a regular cubic lattice. Three types of initial lattices with different ratios of the cell adges parallel and perpendicular to the magnetic field are considered. These initial lattices correspond to three types of distribution of magnetic particles inside an elastomer: isotropic, chain-like and plane-like distributions. It is shown that interaction between the magnetic particles results in the contraction of an elastomer in the direction of the applied homogeneous magnetic field for all structures considered. Similar to the previous studies [1–3], we show that the shear modulus G increases for all types of distribution of magnetic particles with the increase of magnetic field. On the other side, we show that the Young modulus E decreases for the chain-like distribution and increases for the plane-like distribution of magnetic particles with the increase of magnetic field. The moduli G and E are calculated at the strain corresponding to the minimum of free energy. Thus, contrary to the previous studies [1–3], we take into account the influence of the magnetostriction effect on mechanical properties of the magneto-sensitive elastomers.

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[1] Jolly M., Carlson J., Muñoz B., Smart Mater. Struct., 1996, **5**, 607–614.
[2] Davis L., J. Appl. Phys., 1999, **85**, 3348–3351.
[3] Zhu Y.-S., Gong X.-L., Dang H., Zhang X.-Z., Zhang P.-Q., Chin. J. Chem. Phys., 2006, **19**, 126–130.

Dynamics at barriers in bidirectional two-lane exclusion processes

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A two-lane exclusion process is studied where particles move in the two lanes in opposite directions and are able to change lanes. The focus is on the steady state behavior in situations where a positive current is constrained to an extended subsystem (either by appropriate boundary conditions or by the embedding environment) where, in the absence of the constraint, the current would be negative. We have found two qualitatively different types of steady states and formulated the conditions of them in terms of the transition rates. In the first type of steady state, a localized cluster of particles forms with an anti-shock located in the subsystem and the current vanishes exponentially with the extension of the subsystem. This behavior is analogous to that of the one-lane partially asymmetric simple exclusion process, and can be realized e.g. when the local drive is induced by making the jump rates in two lanes unequal. In the second type of steady state, which is realized e.g. if the local drive is induced purely by the bias in the lane change rates, and which has thus no counterpart in the one-lane model, a delocalized cluster of particles forms which performs a diffusive motion as a whole and, as a consequence, the current vanishes inversely proportionally to the extension of the subsystem. The model is also studied in the presence of quenched disordered, where, in case of delocalization, phenomenological considerations predict anomalously slow, logarithmic decay of the current with the system size in contrast with the usual power-law.

Resummed thermodynamic perturbation theory for central force associating potential. Multi-patch models

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A resummed thermodynamic perturbation theory for associating fluids with multiply bondable central force associating potential [1,2,3] is extended to account for the presence of several attractive sites. We consider a simple multi-patch model for associating fluids. The model is represented by the hard-sphere system with several circular attractive patches on the surface of each hard-sphere. Resummation is carried out to account for the blocking effects, i.e., when the bonding of a particle restricts (blocks) its ability to bond with other particles. Closed form analytical expressions for thermodynamical properties (Helmholtz free energy, pressure, internal energy, and chemical potential) of the model with arbitrary number of doubly bondable patches at all degrees of the blockage are presented. In the limiting case of total blockage, when the patches on the particles become only singly bondable, our theory reduces to Wertheim's thermodynamic perturbation theory for polymerizing fluids [4]. To validate the accuracy of the theory we compare its predictions to exact values, for the thermodynamical properties of the system, as determined by Monte Carlo computer simulations. In addition we compare the fraction of multiply bonded particles with different number of patches and at different values of the density and temperature. Very good agreement between predictions of the theory, corrected for ring formation, and Monte Carlo computer simulation values was found in all cases studied.

[1] Y.V. Kalyuzhnyi, G. Stell, Mol.Phys., 1993, **78**, 1247.
[2] Y.V. Kalyuzhnyi, I.A. Protsykevytch, P.T.Cummings, EPL, 2007, **80**, 56002.
[3] Y.V. Kalyuzhnyi, H. Docherty, P.T. Cummings, J. Chem. Phys., 2010, **133**, 044502.
[4] M.S. Wertheim, J. Chem. Phys., 1987, **87**, 7323.

Power laws and critical exponents in n-vector models

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Goldstone mode singularities and critical exponents in the φ^4 model and corresponding n–vector models are considered within the approach called the GFD (grouping of Feynman diagrams) theory [1,2], which is proposed as an alternative to the perturbative renormalization group (RG) treatment. Monte Carlo (MC) evidences [3,4], completed by the most recent simulation results, support the statement of the GFD theory [2] that the Goldstone mode power–law singularities below the critical point are described by certain nontrivial exponents. We have tested also the critical–point singularities and critical exponents found within this approach [1]. A non-perturbative proof concerning corrections to scaling in the two–point correlation of the φ^4 shows that predictions of the GFD theory rather than those of the perturbative RG theory can be correct. We find that the recent MC data for the 3D Ising model ($n = 1$) on very large lattices (up to linear size $L = 1536$) can be well fit with the critical exponents $\eta = \omega = 1/8$ and $\nu = 2/3$, proposed by certain general conjecture made within the GFD theory. We demonstrate also that the known very accurate experimental specific heat data, obtained in zero–gravity conditions very close to the λ–transition point in liquid helium, can be well described by an expansion in powers of $t^{-\alpha}$ with the critical exponent $\alpha \approx -1/13$, estimated as a fit parameter at very small reduced temperatures t. It confirms our conjecture at $n = 2$.

[1] J. Kaupužs, Ann. Phys. (Leipzig), 2001, **10**, 299.
[2] J. Kaupužs, Prog. Theor. Phys,. 2010, **124**, 613.
[3] J. Kaupužs, R.V.N. Melnik, J. Rimšāns, Commun. Comput. Phys., 2008, **4**, 124.
[4] J. Kaupužs, R.V.N. Melnik, J. Rimšāns, Phys. Lett. A, 2010, **374**, 1943.

Gini index for measuring the statistical heterogeneity

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The level of societies' egalitarianism is one of the important characteristics, which enables to estimate the socio-economic development of the country. There is a need for adequate statistical tools and information to help you explore the degree of statistical heterogeneity. Social inequality is a phenomenon that is difficult to be measured, but still the population differentiation in terms of income (expenses) you can explore using statistical indices (indices of relative inequality). They provide an opportunity to assess the level of differentiation and partially answer the question of how equal or unequal is the distribution of income (expenses) in the country. Well-known indices of relative inequality are the Gini index, the Pietra index, the Atkinson index, the Theil index and some others.

However, almost all international statistical agencies and organizations use to describe inequality Gini index, which is the simplest and most obvious index of income inequality. This economic indicator takes values in the unit interval and measures societies' egalitarianism.

In this work we present the new method of the computation of the Gini index, which based on the geometric meaning of this index. This approach uses the distribution of population by income (expenses). In addition, the formula for assessment of accuracy index is received. These formulas are implemented to calculate the Gini index for Ukraine and Lviv region for years 2008-2010. The obtained results are compared with results obtained by the methodology of calculating the Gini index by the State Statistics Committee of Ukraine.

Stochastic effects at pattern formation processes during ion-beam sputtering

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We study pattern formation processes in anisotropic system governed by the Kuramoto-Sivashinsky equation with multiplicative noise as a generalization of the Bradley-Harper model for ripple formation induced by ion bombardment. In our approach we take into account fluctuations for an angle of incidence of arriving ions. In the framework of such approach dynamics of the height field describing the surface target satisfies the Kuramoto-Sivashinsky equation with fluctuating erosion rates. It allows us to consider stochastic scenario for pattern formation where secondary ion beam characteristics such as dispersion of angle of incidence and the correlation scale of its fluctuations can play crucial role in surface morphology change.

For both linear and nonlinear systems we study noise induced effects at ripple formation. The corresponding dynamical phase diagram in the plane dispersion of angle of incidence versus correlation scale of its fluctuations is obtained to show possibility of the pattern formation control by variation of secondary ion beam characteristics. Considering height-height correlation functions dynamics of the surface morphology change we discuss scaling behavior of the surface growth and roughness characteristics. It was found that introduction of the multiplicative noise related to fluctuations in the angle of incidence can accelerate surface growth where a nonlinear regime appears. We have found that there are sets of growth and roughness exponents describing transition from linear to nonlinear regime. Both growth and roughness exponents depend on the secondary ion beam characteristics.

Features of dynamical properties of liquid polyvalent metals near melting point: ab initio molecular dynamics study

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Dynamical properties of bulk liquid Indium and its surface were studied in IXS-experiments [1], but so far no simulation studies at the same thermodynamic point were performed. Liquid Indium is very difficult for classical molecular dynamics simulations because of problems to represent covalent bonding via two- or three-body effective potentials.

We report an ab-initio simulation study of structure and dynamical properties of liquid Indium at the thermodynamic point of the experimental study [1]. Our calculations were performed with ab-initio package VASP [2]. We report pair distribution function and running integration numbers, angle distribution function, velocity autocorrelation function and density of electronic states for liquid bulk Indium. From calculated velocity autocorrelation function and mean-square displacements we were able to estimate diffusion coefficients.

We have found, that there is a tendency in liquid In to formation some kind of dimers or small chains, that follows from the bond-angle distribution function. Such a tendency is known from the literature to exist in liquid Ga.

[1] H. Reichert, F. Bencivenga, B. Wehinger, M. Krisch, F. Sette, H. Dosch, Phys. Rev. Lett., **98**, 2007, 096104.
[2] G. Kresse, J. Furthmuller, Comput. Mat. Sci., **6**, 1996, 15.

Chemical potential of semi-infinite jellium

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Chemical potential of electron subsystem of metal has essential value for building consistent theory of many-electron systems. This characteristic is necessary for correct calculation structural and thermodynamic properties of metal, in particular, work function, surface energy, etc.

Proceeding from the

$$N = -\frac{\partial \Omega}{\partial \mu}$$

(N is the number of electrons, Ω is the grand thermodynamic potential of electron subsystem received in [1]) nonlinear algebraic equation for the chemical potential μ electron subsystem of semi-infinite jellium is obtained.

This equation for the chemical potential μ in the case of low temperatures ($\beta\mu \gg 1$) for different models of the surface potential [1,2] is solved numerically. An influence of parameters of the model surface potentials on the chemical potential μ are investigated.

[1] Kostrobij P.P., Markovych B.M. Condens. Matter Phys., 2003, **6**, 347.
[2] Kostrobij P.P., Markovych B.M. Condens. Matter Phys., 2008, **11**, 641.

Entanglement entropy of the random transverse-field Ising model in higher dimensions

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The entanglement entropy of quantum many-particle systems is extensively studied, especially around quantum critical points, where phase transitions take place. The entanglement in the $|\Psi\rangle$ ground state can be quantified by the von Neumann entropy between an $\mathcal{A}$ part and the rest of the system ($\mathcal{B}$) as $\mathcal{S}_\mathcal{A} = -\mathrm{Tr}_\mathcal{A}(\rho_\mathcal{A} \log \rho_\mathcal{A})$ in terms of the reduced density matrix $\rho_\mathcal{A} = Tr_\mathcal{B}|\Psi\rangle\langle\Psi|$. The entanglement entropy of a subsystem with linear size ℓ is usually expected to scale with the area of the boundary of the subsystem, $\mathcal{S}(\ell) \sim \ell^{d-1}$, known as the *area law*. On the contrary, as now well understood in 1 dimensional pure and disordered systems, the critical entanglement entropy shows logarithmic divergence $\mathcal{S}(\ell) \sim \ln \ell$ in 1D. In higher dimensional interacting systems, the characterization of the entanglement entropy turned out to be rather too difficult, resulting in almost complete lack of results. One exception is the random transverse-field Ising model, where the strong disorder renormalization group (SDRG) technique enabled to study 2 dimensional critical systems up to about ten thousand spins. For the time being two different interpretations of the data are available. Lin *et al.* (2007) observed a double-logarithmic multiplicative factor to the area law, whereas Yu *et al.* (2008) argued to have only a subleading logarithmic term to the area law. By using our efficient SDRG algorithm, we could analyze the critical behaviour up to several million spins, not only in 2, but also in 3 and 4 dimensions. A related question in higher dimensions is, whether the entanglement entropy has a maximal value at the critical point, indicating the location of the phase transition, as found in 1D. In order to test this, we also studied the von Neumann entropy outside the critical point in 2, 3 and 4 dimensions.

The equation of state of the n-vector model

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The critical behavior of the three-dimensional n-vector model in the presence of an external field is investigated. Analytical description is performed with the collective variables method in the framework of the ρ^4 model approximation at the microscopic level without any adjustable parameters. Recurrence relations of the renormalization group as functions of the external field and temperature were found. Analytical expression for the free energy of the system at temperatures $T > T_c$ and different values of n was obtained. The equation of state of the n-vector model for the general case of small and large external fields was written. Explicit form of the correspondent scaling functions for different values of the order parameter was derived. Obtained results are in qualitative agreement with the data of Monte Carlo simulations.

Quenched thermodynamic states of the Ising model on random graphs

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It is proven that the zero external field Ising ferromagnet on a scale-free graph with $p_k \sim k^{-\lambda}$ and $\lambda \leq 3$ can be in a paramagnetic state at finite temperatures, which contradicts the common belief that this property holds only if $\sum_k p_k k^2 < \infty$. Namely, we prove this result for the genealogic tree of a non-extinct Galton-Watson process with $\sum_k p_k k \ln k < \infty$. The proof consists in showing that the magnetization M vanishes if $2\beta J < \ln(a/a-1)$, where $a = \sum_k k p_k$. It is based on the Kesten-Stigum theorem and on a special representation of M.

Ferromagnetism in spin subsystem hybridized with conduction band in Anderson-Hubbard-type model

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Magnetic ordering mechanisms in spin subsystem of an analogue of Anderson-Hubbard model [1] have been studied. Besides the spin-spin interactions and strong on-site Coulomb interaction, the model takes into account the hybridization with conduction band which results in the indirect hopping and indirect exchange interaction. Configurational representation of Hamiltonian with Hubbard X-operators describing the localized spin subsystem has been built. On this base the effective Hamiltonian has been constructed for the case of strong Coulomb correlation and classification of effective exchange and effective hopping parameters within the model has been proposed. Magnetization of the localized spin subsystem has been calculated. Our results show that in the considered model the effects of localization are enhanced due to reduced values of indirect hopping integrals in comparison with standard s-d-model. For the ground state in the case of rectangular bare density of states the analytical solution for magnetization as a function of the effective bandwidth, electron concentration and model parameters has been obtained. Criteria for the ferromagnetic ordering stabilization have been found for arbitrary temperatures. Curie temperature for the system with Anderson-Hubbard centers has been calculated numerically for wide range of electron concentrations in different correlation regimes. For the particular case of weak effective exchange, the formula for the Curie temperature reproducing the well-established results has been calculated analytically. It is worth to note that the obtained values of Curie temperature are proportional to conduction band width, though the ferromagnetic ordering is stabilized by the indirect exchange interaction. The region of electron concentrations favorable for ferromagnetic ordering stabilization depends substantially on hybridization through effective exchange integral.

[1] V.Yu. Irkhin and Yu.P. Irkhin. Electronic Structure, Correlation Effects and Physical Properties of d- and f- Metals and their Compounds. Cambridge International Science Publishing, 2007.

Field theoretical approach for a nematic fluid: beyond the Maier-Saupe theory

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We use a statistical field-theoretical approach to describe the structure and thermodynamics of a homogeneous anisotropic fluid. The Hamiltonian $H[\rho(\mathbf{r},\Omega)]$ is a functional of field and consists of the ideal entropy and the orientation-dependent interaction:

$$\begin{aligned}\beta H[\rho(\mathbf{r},\Omega)] &= \beta H^{entr}[\rho(\mathbf{r},\Omega)] + \beta H^{int}[\rho(\mathbf{r},\Omega)] \\ &= \int \rho(\mathbf{r},\Omega)\left[\ln\frac{\rho(\mathbf{r},\Omega)}{\rho_{ref}} - 1\right] d\mathbf{r}d\Omega \\ &+ \frac{1}{2}\int \nu(r_{12},\Omega_1\Omega_2)\rho(\mathbf{r_1},\Omega_1)\rho(\mathbf{r_2},\Omega_2)d\mathbf{r_1}d\mathbf{r_2}d\Omega_1 d\Omega_2\end{aligned}$$

The intermolecular potential $\nu(r_{12},\Omega_1\Omega_2)$ has the form

$$\nu(r_{12},\Omega_1\Omega_2) = \frac{A_0}{r_{12}}e^{-\alpha_0 r_{12}} + \frac{A_2}{r_{12}}e^{-\alpha_2 r_{12}}P_2(\cos\Omega_{12}),$$

where $P_2(\cos\Omega_{12})$ is the second order Legendre polynomial of the relative molecule orientations.

Our assumption is that the partition function can be expressed exactly as a functional integral according to

$$\Xi\left[\rho(\mathbf{r},\Omega)\right] = \int D\rho(\mathbf{r},\Omega)\exp\{-\beta H[\rho(\mathbf{r},\Omega)]\}$$

Based on this approach, in the mean field approximation we retrieve the standard Maier-Saupe theory for liquid crystals. In the Gaussian approximation we obtain analytical expressions for the correlation functions, the elasticity constants, and the free energy. Subsequently we find corrections due to fluctuations and show that density now contains Legendre polynomials of higher orders. We also use Ward symmetry identities to set a simple condition for the correlation functions.

Low-temperature properties of frustrated classical spin chain near the ferromagnet-helimagnet transition point

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Last year much attention has been paid to the 1D $J_1 - J_2$ Heisenberg model that exhibit frustration. Its Hamiltonian has a form

$$H = J_1 \sum \mathbf{S}_n \mathbf{S}_{n+1} + J_2 \sum \mathbf{S}_n \ \mathbf{S}_{n+2} \,, \qquad (1)$$

where $J_1 < 0$ is the ferromagnetic (NN) coupling while $J_2 > 0$ is the antiferromagnetic (NNN) interaction. This model is basic one for the description of magnetic properties of recently synthesized edge-shared cuprate chain compounds. The model is characterized by the frustration parameter $\alpha = J_2/|J_1|$. The ground state of the model is ferromagnetic for $\alpha < 1/4$. At $\alpha = \alpha_{\rm c} = 1/4$ the ground state phase transition to the singlet phase with helical spin correlations takes place. Remarkably, this transition point does not depend on a spin value, including the classical limit $s = \infty$. The interesting question related to this model is the influence of the frustration on the low-temperature thermodynamics near the transition point. We study this problem for the classical version of the model (1). The calculation of the partition and spin correlation functions is reduced to quantum mechanics problem of a particle in a potential well. It is shown that exactly in the transition point at $T \to 0$ the correlation length $l_{\rm c} \sim T^{-1/3}$ and zero field susceptibility $\chi \sim T^{-4/3}$ in contrast with the Heisenberg ferromagnet ($\alpha = 0$) where $l_{\rm c} \sim T^{-1}$ and $\chi \sim T^{-2}$. Corresponding numerical factors for $l_{\rm c}$ and χ are found. The behavior of the low-temperature susceptibility in the helical phase near the transition point is described by the universal dependence of the scaling variable $t = T/(\alpha - \alpha_{\rm c})^{3/2}$. In particular, $\chi(T)$ has a maximum at $T_{\rm m} \sim (\alpha - \alpha_{\rm c})^{3/2}$ and $\chi_{\rm m} \sim (\alpha - \alpha_{\rm c})^{-2}$. The obtained dependence $\chi(T)$ is in qualitative agreement with that observed in edge-shared cuprates with α close to $\alpha_{\rm c}$.

Magnetization processes at low temperatures for two frustrated quantum Heisenberg antiferromagnets

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We consider the quantum Heisenberg antiferromagnet on the frustrated two-leg ladder and bilayer lattices to examine magnetization processes at low temperatures for these spin models. Our approach is based on a lattice-gas description of the low-energy degrees of freedom which can be elaborated for a certain class of frustrated quantum Heisenberg antiferromagnets in the so-called strong-coupling regime [1]. For both considered models these emergent discrete degrees of freedom implicate a close similarity of the quantum models to the classical lattice gas with finite nearest-neighbor repulsion or, equivalently, the Ising antiferromagnet in a uniform magnetic field. The main focus of our study is the magnetization curves $M(h)$ at low temperatures, which can be obtained experimentally. We also calculate the susceptibility $\chi(h) = \partial M(h)/\partial h$ at low temperatures, which is also often reported in experimental papers. In the one-dimensional case we obtain analytical results for thermodynamically large systems using the transfer-matrix approach. In the two-dimensional case we perform classical Monte Carlo simulations for systems up to 100×100 sites. We discuss in detail the low-temperature uniform magnetization and susceptibility within the frames of the lattice-gas description.

Some further details can be found in [1].

[1] Derzhko O., Krokhmalskii T., Richter J., Phys. Rev. B, 2010, **82**, 214412.

Global isomorphism between the Lennard-Jones fluids and the Ising model

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The simple geometrical picture of global isomorphism between Ising model (Lattice Gas) and simple fluid is proposed. It is naturally incorporates two classical linear laws know more than a century for the molecular liquids. They are the linear character of the diameter for the binodal

$$n_{\rm d} = \frac{n_{\rm l} + n_{\rm g}}{2n_{\rm c}} = 1 + A\,\frac{T_{\rm c} - T}{T_{\rm c}} + \cdots$$

and the linear character of the Zeno-line (unit compressibility line $Z = P/(n\,T) = 1$) also called Batschinski law. The correct definition of the Zeno-element is given and its relation with the locus of the critical point is derived within this approach. We show that the liquid-vapor part of the phase diagram of the molecular fluids can be described as the isomorphic image of the phase diagram of the Lattice Gas. The relations between the thermodynamic functions are obtained. The position of the critical points of the fluids of the Lennard-Jones type are determined basing on the scaling symmetry. In case of two dimensions we use the exact Onsager result to construct the binodal of the corresponding Lennard-Jones fluid and compare it with the results of the simulations. In the three dimensional case we use available numerical results for the Ising model for the corresponding mapping. As a sequence the explanation of the well known fact about "global" cubic character of the coexistence curve of the molecular fluids is proposed. The microscopic approach to the construction of the isomorphism based on the Hamiltonian is discussed.

Mutual diffusion and partial conductivities in multicomponent ionic liquids

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Starting from the rigorous expressions, derived for the generalized transport coefficients of a multi-component fluid, we obtained the exact relation for (k, ω)-dependent partial conductivities of a multicomponent ionic mixture [1].

For a simpler case of a charge-symmetric binary molten salt such kind of relations was discovered experimentally by Sundheim [2] more than 50 years ago and is known as the "universal golden rule". Later were made several attempts to derive the relations for partial ionic conductivities in charge-symmetric binary and three-components pseudo-binary molten salt using the equations of motion, the Langevin equation as well as molecular dynamics simulations (see, e. g. [3]).

In the case of ν-component system of charged particles with m_α and q_α being masses and charges of ions in the α species, respectively, the relations derived for partial conductivities $\sigma_\alpha(k, \omega)$ can write as follows:

$$\sum_{\alpha=1}^{\nu} \frac{q_\alpha}{m_\alpha} \sigma_\alpha(k, \omega) = 0.$$

If the case of an ionic mixture in electro-neutral solvent is considered one gets more complicate expression

$$\sum_{\alpha=1}^{\nu} \frac{q_\alpha}{m_\alpha} \sigma_\alpha(k, \omega) = -D_{MQ}(k, \omega),$$

where $D_{MQ}(k, \omega)$ is the generalized transport coefficient that describes the diffusive mass and charge cross-correlations between electro-neutral solvent and ionic components of mixture [1].

[1] I.M. Mryglod, V.M. Kuporov, Cond. Matt. Phys., 2010, **13**, 43602.
[2] B.R. Sundheim, J. Phys. Chem., 1956, **60**, 1381.
[3] T. Koishi, S.Kawase, S.Tamaki, J. Chem. Phys., 2002, **116**, 3018.

Slow dynamics of colloids in porous media: the roles of confinement and caging

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Using molecular dynamics simulations, we have studied the dynamic arrest of a dense hard-sphere fluid moving in a disordered configuration of hard-sphere obstacles. The high density and the quenched disorder lead to two distinct dynamic arrest mechanisms-confinement and caging-that can also be observed for instance in the movement of proteins in cytoplasm. We have investigated the specific case of "quenched-annealed" systems in which the obstacles are quenched from an equilibrium fluid, and the fluid particles are subsequently inserted at arbitrary positions. Upon varying the two control parameters of the system (the volume fractions of the fluid and of the obstacles) we unveiled scenarios of both discontinuous and continuous dynamic arrest, anomalous diffusion, as well as a decoupling of the time scales for the relaxation of the single-particle and the collective correlators of the system. Our observations are consistent with many predictions by a recent extension of mode-coupling theory to systems with quenched disorder. In order to elucidate the microscopic origin of the observed dynamic arrest scenarios, we performed a Delaunay decomposition of the pore structure. We were thus able to distinguish between particles that are "free" (located in the void percolating through space) and "trapped" (confined in a void of finite volume). For these two classes of fluid particles we separately evaluated various dynamic correlators such as the single-particle intermediate scattering function, the mean-squared displacement and its logarithmic derivative, as well as the self part of the van Hove function. We thereby demonstrated that the free and the trapped particles exhibit nontrivial differences in their dynamic properties, which may serve as a basis for more refined theories.

Dielectric, piezoelectric and elastic properties of quasione-dimensional $Cs(H_{1-x}D_x)_2PO_4$ ferroelectrics

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Within the framework of the proposed modified proton ordering model for quasione-dimentional CsH_2PO_4 type ferroelectrics with hydrogen bonds, that takes into account linear over strains ε_6 and ε_4 contributions to the proton subsystem energy, and using a four-particle cluster approximation with taking into account short-range and long-range interactions between protons on short hydrogen bonds we have calculated and studied spontaneous polarization, longitudinal static dielectric permittivities of mechanically free and clamped crystals, coefficients and constants of piezoelectric strain and stress, and also elastic constants of these crystals.

Dynamic characteristics of the crystals are explored within a nonequilibrium statistical operator method with taking into account dynamics of strains via Newtonian equations of motion. In the case of frequency-independent kinetic parameters these results are shown to be agreement with those obtained by us in the frames of Glauber method.

A thorough numerical analysis of the obtained results is performed. Phenomena of piezoelectric resonance in some frequency region in the low-temperature phase is described. It is shown, that at proper set of the model parameters it is proper description of experimental data for thermodynamic and dynamic characteristics of $Cs(H_{1-x}D_x)_2PO_4$ ferroelectrics.

Spin-1/2 asymmetrical diamond Ising-Heisenberg chain

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The ground state and thermodynamics of the spin-1/2 asymmetrical diamond Ising-Heisenberg chain are considered. For the XYZ anisotropic Heisenberg interaction exact results for free energy, entropy, specific heat, magnetization and magnetic susceptibility are obtained by using the method of decoration-iteration transformation.

In the case of antiferromagnetic Ising and XXZ Heisenberg interactions the ground state, field and temperature dependencies of magnetization, magnetic susceptibility, and specific heat are investigated. The influence of geometric frustration and quantum fluctuations on these characteristics is studied. It is shown that in the ground state the strong enough quantum fluctuations remove the effect of geometric frustration on the Heisenberg bond. An increase of the quantum fluctuations shifts the high-temperature magnetization curve of the Heisenberg (Ising) subsystem to the region of higher (lower) magnetization. Consequently, the total high-temperature curve shifts to the higher magnetization. The zero-field specific heat of the system may have two additional low-temperature peaks.

Everything about statistics of the Ising model

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The Zipf-Mandelbrot power law and it's correspondence with the inhomogeneity of the system has been considered. We describe the statistical distributions of the domain masses in the two dimensional Ising model beyond and near the phase transition induced by the temperature. The statistical distribution of domain masses near the critical point appears to be of the Pareto type. For the small domain masses we observe the Gaussian type number distributions.The relation to the hyperbolic distribution functions and the Shannon entropy is shown also.

[1] Lukierska-Walasek K., Topolski K., Computational Methods in Science and Technology, 2010, **(16)2**, 173–176.
[2] Lukierska-Walasek K., Topolski K., Rev. Adv. Mater. Sci., 2010, **23**, 146.
[3] Harremoes P., Topsoe F., Entropy, 2001, **3**, 191–226.

Networks in mythology

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Although qualitative notions of universality exist within the field of comparative mythology, there is no classification system to facilitate comparison of myths. The concept of universality also lies at the heart of statistical physics and network theory. Here, we apply network theory to a variety of mythologies to quantify their characteristics. In this way, myths can be classified and compared across different cultures. We also compare mythological networks to other networks, both actual and fictitious in an effort to discover where they are positioned along the spectrum from the real to the imaginary.

Magnetic friction – from Stokes to Coulomb

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Friction forces in purely magnetically interacting systems have been neglected for a long time, although they offer a broad spectrum of phenomena as recent studies show. For example, on the one hand analytical and Monte Carlo calculations of systems, which are moved with respect to each other tangentially, in the Ising [1, 2] and the Potts [3] model show that the friction force as function of velocity v gets constant in the $v \to 0$ limit ("Coulomb friction"). On the other hand simulations of a magnetic tip scanning a Heisenberg ferromagnet yield a friction force proportional to the velocity ("Stokes friction", [4, 5]).

We present results of spin chains in both, the Ising and the Heisenberg model, scanned by a tip. The systems undergo Metropolis spin-flip dynamics for the Ising case and precessional Landau-Lifshitz-Gilbert dynamics for the Heisenberg case. For each system class we observe both Coulomb and Stokes friction. The underlying regime is determined by the field characteristics and the velocity. In between the regimes we observe a cross-over at a corresponding velocity. Analogous to dry friction, the occurrence of Coulomb friction is linked to the existence of two separate timescales, defined by the scanning velocity and the spin relaxation time.

[1] D. Kadau, A. Hucht and D.E. Wolf, Phys. Rev. Lett., 2008, **101**, 137205.
[2] A. Hucht, Phys. Rev. E, 2009, **80**, 061138.
[3] F. Iglói, M. Pleimling and L. Turban, 2010, arXiv:1010.0738.
[4] C. Fusco, D.E. Wolf and U. Nowak, Phys. Rev. B, 2008, **77**, 174426.
[5] M.P. Magiera, L. Brendel, D.E. Wolf and U. Nowak, EPL, 2009, **87**, 26002.

Contribution of H-bond vibrations to the heat capacity of water

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The anomalously large value of the heat capacity of liquid water is discussed. Comparing the temperature dependencies of the heat capacities for water with that for argon and hydrogen sulfide we separate the contributions of the translational and rotational degrees of freedom. The residual part is considered as one caused by specific contributions of transversal vibrations of H-bonds. The estimate for the number of H-bonds per molecule, obtained from the analysis of this contribution, is in quite good agreement with similar estimates following from the analysis of the specific volume and heat of evaporation as well as the kinematic shear viscosity.

This work is devoted to the consecutive analysis of different contributions to the heat capacity of liquid water. The main attention is focused on the correct separation of the contributions to C_v caused by the translational and rotational degrees of freedom. For this purpose the careful comparison of the heat capacities of water and argon and hydrogen sulfide is carried out. The role playing by the thermal excitations of the H-bond network in water is studied.

Localized states on triangular traps and low-temperature properties of some strongly correlated lattice models

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We consider the antiferromagnetic Heisenberg model and the repulsive Hubbard model on two N-site one-dimensional lattices (the double-tetrahedra chain and the frustrated three-leg ladder), both of which support dispersive one-particle states corresponding to localized-magnon or localized-electron states on triangular trapping cells. Following the previous studies on localized-magnon and localized-electron states (see [1], [2] and references therein) we calculate the degeneracy of the ground states in the subspaces with $n \leq n_{\max}$, $n_{\max} \propto N$ magnons or electrons. Moreover, we calculate the contributions of these states to thermodynamic quantities. We also calculate the contribution to thermodynamics of low-lying excited states. A new feature of the localized states on triangular traps is related to the chirality of the triangles. In our study we examine the effect of extra interspin or interelectron interactions which lift the degeneracy owing to the chirality of the triangles. Small symmetry-breaking interactions lead to appearance of effective spin-1/2 XY chains which describe the low-energy degrees of freedom of the initial strongly correlated lattice models.

For some further details see Ref. [3].

[1] O. Derzhko, T. Krokhmalskii, J. Richter, Phys. Rev. B, 2010, **82**, 214412.
[2] O. Derzhko, J. Richter, A. Honecker, M. Maksymenko, R. Moessner, Phys. Rev. B, 2010, **81**, 014421.
[3] M. Maksymenko, O. Derzhko, J. Richter, Acta Physica Polonica A (to appear); Preprint ICMP-10-08E.

Transition to ferromagnetic ground-states in the two-dimensional Tasaki-Hubbard model

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We consider the N-site Hubbard Hamiltonian on the 2D Tasaki lattice [1] to discuss the flat-band Mielke-Tasaki ferromagnetism [2]. Due to localized nature of the lowest-energy one-electron states, many-electron ground states can be constructed for the number of electrons $n \leq \mathcal{N} = N/4$ [1,2]. We have checked this construction by the exact diagonalization for finite systems with $N = 24, 30, 48$ and calculating ground-state degeneracies $g_{\mathcal{N}}(n)$ for $n \leq \mathcal{N}$. In all cases ED data coincide perfectly with predictions based on simple combinatorial arguments. In contrast to the 1D Tasaki-Hubbard model, many-electron ground states cannot be mapped onto spatial configurations of hard-core objects [3], but one can use a percolation representation introduced in Ref.[2]. Various ground-state expectation values (e.g., of the square of the total spin of electrons $\mathbf{S}^2$) can be presented in terms of expectation values in a percolating system. Moreover, because of the Kramers degeneracy of independent clusters we face a *weighted* site-percolation problem on the square-lattice. We adjust the Hoshen-Kopelman and Newman-Ziff algorithms to simulate the weighted site-percolation problem and to calculate $\langle \mathbf{S}^2 \rangle$. Our simulations give evidence that ground-state ferromagnetism occurs if $n/\mathcal{N}$ exceeds the critical value - higher than the percolation threshold 0.592746 for standard percolation on a square lattice.

[1] H. Tasaki, Phys. Rev. Lett., 1992, **69**, 1608.
[2] A. Mielke, H. Tasaki, Commun. Math. Phys., 1993, **158**, 341.
[3] O. Derzhko, J. Richter, A. Honecker, M. Maksymenko, R. Moessner, Phys. Rev. B, 2010, **81**, 014421.

Collective modes in a dusty plasma

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A consistent statistical description of kinetics and hydrodynamics of a dusty plasma [1] is carried out by means of the Zubarev nonequilibrium statistical operator method. The consideration is based on the partial dynamics of each of the components with out taking into account for ionization processes and atom adsorption on the surface of dust particles. We considered the nonequilibrium state of a system when the subsystem of electrons, ions and atoms is in hydrodynamic state but dust particles whose mass and charge can alter remain in kinetic state.

The nonequilibrium statistical operator is constructed and with its help a set of generalized transport equations for a consistent description of kinetics of dust particles and hydrodynamics of electrons, ions and neutral atoms is obtained. For the case of weak nonequilibrium processes by means of perturbation theory for collective modes [2] spectrum of collective excitations of dusty plasma is investigated.

[1] M.V. Tokarchuk, B.B. Markiv, Fiz. Zbirnyk, 2008, **7**, 100 (in Ukrainian).
[2] T.M. Bryk, I.M. Mryglod, Condens. Matter Phys., 2008, **11**, 139.

Biaxial nematic liquid crystals: Green functions and polarization features of acoustic waves

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In the report the results of investigation of biaxial (with ellipsoidal and discoidal molecules) nematic liquid crystals are presented. The work is based on Hamiltonian approach which is characterized by establishment of the set of reduced description parameters, macroscopically full specifying investigated physical systems, Hamiltonian as the function of these parameters and obvious kind of Poisson brackets for the whole set of reduced description parameters. For the adequate description of biaxial nematic liquid crystals, besides densities of momentum, entropy and number of particles, additional dynamic parameters are introduced. They are two unit vectors of spatial anisotropy and three conformational degrees of freedom (lengths of molecule axes and an angle between them). On the basis of the approach, developed by us, the nonlinear dynamic equations taking into account molecules size and shape are derived. The acoustic spectra of collective excitations for investigated condensed matters are found out and it is shown, that taking into account molecules size and shape leads to the appearance of one up to three sounds in biaxial nematics already in adiabatic approximation. The polarization features of acoustic waves in considered liquid crystals are investigated. The nonlinear dynamic equations for the considered liquid crystals with regard to the anisotropy axes and conformational parameters in external alternating field are derived and the kind of sources in the dynamic equations corresponding to this field is determined. The analytic expressions for low-frequency asymptotics of Green functions are obtained. Asymptotics of Green functions in the region of small wave vectors and frequencies essentially depend on the character of spatial anisotropy of considered condensed matter.

Vapour-liquid phase diagram of long-range Yukawa fluids

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In their paper Caillol et al [Mol. Phys., 2007, **105**, 1813.] have reported an extensive Monte Carlo study of the liquid/vapor coexistence in the long-range attractive Yukawa fluid. In the same study these authors have shown that two theoretical approaches, namely, the self-consistent Ornstein-Zernike equation (SCOZA) and the hierarchical reference theory (HRT) perform extremely well in reproducing these computer simulation data. At the same time, an optimized mean field theory (OMF) while yielding the exact result in the limit of infinite range of the potential, still deteriorates with decreasing interaction range. In present work we have shown that recently proposed an augmented van der Waals theory builded up on the short-range attractive Yukawa fluid performs as well as both advanced theoretical approaches, SCOZA and HRT.

Comparison of grafted and non-grafted polymer adsorption in different ensembles

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After we recently found first-order like signatures in the microcanonical entropy at the adsorption transition of a finite single free polymer in good solvent [1], and knowing that many studies on polymer adsorption in the past have been performed for grafted polymers, we attempt a comparison of the thermodynamic behavior for both cases with the present work. This comparison not only covers the adsorption transition but all transitions a coarse-grained off-lattice model undergoes close to an attractive substrate are analysed for both cases and compared over a wide parameter range. Due to the impact of grafting especially on the translational but also on the conformational entropy of desorbed chains, the adsorption transition is affected the strongest. The results are obtained by a combined canonical and microcanonical analysis of parallel tempering Monte Carlo data.

[1] M. Möddel, W. Janke, and M. Bachmann, Phys. Chem. Chem. Phys., 2010, **12**, 11548.

Mitsui model with diagonal strains: description of external pressures influence and thermal expansion of Rochelle salt

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We elaborate a modification of the two-sublattice Mitsui model that takes into account a coupling with diagonal components of the lattice strain tensor ε_i $(i = 1, 2, 3)$ and with the shear strain ε_4. The developed model is used to describe the influence of thermal expansion, as well as of external pressures that do not change the system symmetry (hydrostatic, uniaxial, and biaxial applied along the orthorhombic crystallographic axes of the crystals) on the phase transitions and physical characteristics of Rochelle salt crystals.

We obtain expressions for the related to those strains dielectric, thermal, piezoelectric, electrostrictive, and elastic characteristics of Rochelle salt. For description of the dielectric permittivity under hydrostatic pressure near the lower Curie point an expression for the permittivity of a partially clamped crystal is derived. The set of the model parameters is found, providing a satisfactory agreement with the available experimental data for the hydrostatic and uniaxial pressure dependences of the Curie temperatures, temperature dependences of thermal diagonal strains and their anomalous parts induced by the electrostrictive coupling to the spontaneous polarization, specific heat, as well as related to the diagonal strains linear thermal expansion coefficients, elastic constants, electrostriction constants, and piezoelectric coefficients of Rochelle salt. It is also shown that the physical characteristics related to the shear strain are better described by the present model than by the Mitsui model with the shear strain only.

An attempt of scientometric analysis of Chornobyl-related papers

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In our study we analyze how does an academic community react on a particular urgent task which abruptly arises and poses also scientific problems. To this end, we have chosen to examine a body of research strictly concerning Chornobyl disaster that occurred on 26 April 1986 in Chornobyl (Chernobyl), Ukraine, at the nuclear power plant and by now is considered the worst nuclear power plant accident in history.

Our objective is to analyze several scientometric features of Chornobyl-related research: its multidisciplinary landscape, grows rate, and collaboration strategy. To this end, we analyze data about the papers that appeared in scientific journals since 1986 using the *Scopus* database [1] and the Ukrainian bibliographic database *Ukrainika naukova* [2]. In order to quantify our analysis, we measured distribution of papers between different scientific fields, constructed coauthorship network and defined its main characteristics, calculated growth rates of research in different fields. In particular, our analysis allows to compare contribution of the international community to the Chornobyl-related research as well as integration of Ukraine in the international research on this subject.

[1] http://www.scopus.com.
[2] http://www.nbuv.gov.ua/db/ref_inf.html.

Bose-Fermi-Hubbard model: pseudospin operator approach

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The phase transitions at finite temperature in the systems described by the Bose-Fermi-Hubbard model are investigated in the framework of the selfconsistent random phase approximation. The model takes into account the presence of boson and fermion subsystems and interaction between them. Such type models can be applied for the description of optical lattices, intercalation in crystals and ionic conductivity.

The case of the hard-core bosons is considered and the pseudospin formalism is used. The density-density correlator is calculated in the random phase approximation and the possibilities of transitions from superfluid to supersolid phases are investigated. It is shown that at small values of the bosonic hopping parameter the system undergoes a phase transition from the uniform nonsuperfluid to modulated phase. At increase of the bosonic hopping parameter the phase transition from the superfluid phase to the supersolid phase with a doubly modulated lattice period takes place. The transitions between uniform and charge-ordered phases can be of the second or first order, depending on the system parameters.

Application of SLE(κ, ρ) on the Statistical Models

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Schramm-Loewner Evolution (SLE) is a stochastic process that helps classify critical statistical models using one parameter (κ). To avoid numerical errors in studying the critical curves which start from the real axis and end on it, we have used hydrodynamically normalized SLE (κ, ρ) which is a stochastic differential equation that is hypothesized to govern these curves. We directly verify this hypothesis and numerically apply this formalism to the domain wall curves of the Abelian Sandpile Model (ASM) ($\kappa = 2$) and critical percolation ($\kappa = 6$). We observe that this method is more accurate for analyzing interface loops of statistical models.

Statistical field theory of nonextensive systems

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A field theory is developed for nonextensive statistical systems on the basis of the generating functional

$$Z_q\{u(\mathbf{r},t)\} = \int Z_q\{x\} e_q \left[\int ux \left(Z\{x\} \right)^{q-1} \mathrm{d}\mathbf{r}\mathrm{d}t \right] Dx. \qquad (1)$$

Here, $q \in (0,\infty)$ is deformation parameter; $x(\mathbf{r},t)$ and $u(\mathbf{r},t)$ are fluctuating order parameter and its conjugate field, respectively; $e_q(x) := [1+(1-q)x]^{\frac{1}{1-q}}$ is the Tsallis exponential related to $1+(1-q)x \geqslant 0$. The generating functional (1) represents a generalized Fourier-Laplace transform of the partition functional

$$Z_q\{x(\mathbf{r},t)\} = \frac{2\pi}{2-q} \int e_q \left[-S\{x(\mathbf{r},t)p(\mathbf{r},t)\} \right] Dp \qquad (2)$$

being integral over generalized momentum $p(\mathbf{r},t)$ conjugated to the generalized coordinate $x(\mathbf{r},t)$. Here, the effective action $S = \int \mathcal{L}\mathrm{d}t$ is defined by the Lagrangian

$$\mathcal{L} = p\left(\dot{x} - \nabla^2 x + \frac{\partial V}{\partial x} \right) - \frac{p^2}{2} \qquad (3)$$

with an effective potential $V = V(x)$ being the free energy. Equations of the system evolution within phase space is shown to be non-dependent of the deformation parameter q, whose value determines only the probability to realize phase trajectories

$$P_q\{x(\mathbf{r},t), p(\mathbf{r},t)\} \propto e_q \left[-S\{x(\mathbf{r},t), p(\mathbf{r},t)\} \right].$$

Within the harmonic approach, deformed partition function and moments of the order parameter of lower powers are found. A set of equations for the generating functional is obtained to take into account constraints and symmetry of the statistical system.

Multiple time scale molecular dynamics of complex fluids

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Molecular dynamics (MD) remains one of the most fruitful methods for the investigation of various properties in fluids. This especially concerns complex liquids, such as water, solvated proteins and other collections of biophysical molecules, which are of interest for modern chemistry and medicine. The characteristic feature of these systems is the coexistence of dynamical processes with vastly different time scales. For instance, in water the intramolecular vibrations of atoms relate to the fastest motion, an intermediate time scale arises from the strong short-range intermolecular interactions, while slow dynamics appears due to the weak long-range van der Waals and Coulombic potentials. A lot of multiple time stepping (MTS) approaches have been devised over the years to speed up the MD computations [1]. However, due to the presence of MTS resonance instabilities, the size of the time step in these approaches is limited to relatively small values.

In the current study we propose a novel MTS technique in order to obviate the limitations on the size of the time step in MD simulations of complex fluids. It presents a nontrivial combination of the decomposition operator method with a specific extrapolation of intermolecular interactions complemented by an extended isokinetic Nosé-Hoover chain approach in the presence of translational and orientational degrees of freedom. While the existing multiscale algorithms can increase the outer size of the time step from 5 fs to 100 fs, it is shown on the basis of MD simulations of water that the new technique allows one to significantly overcome this limitation. In particular, now giant time steps of order 500 fs up to 5 ps can be used for studying equilibrium and conformational properties without loss of precision.

The new approach can be applied to more complex models of fluids and their mixtures. It can also be jointed with the integral equation method to further increase the efficiency of the calculations.

[1] I.P. Omelyan, J. Chem. Phys., 2009, **131**, 104101.

Entropic equation of state and scaling functions for spin models on scale-free networks

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Many real world processes may be analyzed applying the methods and tools of statistical mechanics to the corresponding systems. A prototype example is the that of the standard Ising model. However, instead of spins on a regular lattice one considers spins associated with the individuals (nodes) of a social network. The latter model may be used to describe opinion formation processes in society. In this way fundamental equations and laws of statistical mechanics interpreted appropriately may quantitatively describe aspects of social behaviour. In the present work a model with a single order parameter (Ising model) on a scale-free network is analyzed by determining the entropic equation of state and the relative scaling functions. Both are of fundamental importance within the theory of phase transitions and critical phenomena. Here we obtain general scaling functions for the entropy, the constant-field heat capacity, and the isothermal magnetocaloric coefficient near the critical point in scale-free networks. The essential influence of the basic network structure as expressed e.g. by the node degree distribution on the behaviour of the above mentioned quantities is confirmed, extending the principle of universality to systems on scale-free networks.

[1] C. von Ferber, R. Folk, Yu. Holovatch, R. Kenna, and V. Palchykov. Preprint arXiv:1101.3680v1, 2011.

Improvement of Monte Carlo estimates with finite-size scaling at fixed phenomenological coupling

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In the finite-size scaling analysis of Monte Carlo data, instead of computing the observables at fixed Hamiltonian parameters, one may choose to keep a Renormalization-Group invariant quantity, also called phenomenological coupling, fixed at a given value. Within this scheme of finite-size scaling, we exploit the statistical covariance between the observables in a Monte Carlo simulation in order to reduce the statistical errors of the quantities involved in the computation of critical exponents. This method is demonstrated in the Ising model in two and three dimensions.

Gas-liquid coexistence in asymmetric primitive models of ionic fluids

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The gas-liquid coexistence of z:1 asymmetric primitive models is studied using the collective variable based theory. Coexistence-curve data are examined in terms of the corresponding-state variables $\tau^* = |T^* - T_c^*|/T_c^*$ and $\Delta\rho^* = |\rho^* - \rho_c^*|/\rho_c^*$. Calculations are made for 1:1, 2:1, 3:1 valences and for different values of ion size ratio $\lambda = \sigma_+/\sigma_-$ ($\lambda \geq 1$ and $\lambda \leq 1$). We analyze a dependence of the critical amplitude of the coexistence curve and the asymptotic slope of the coexistence-curve diameter on the ion size ratio at a fixed valence. It is shown that the both characteristics take maximum values in the equisize case and demonstrate a nonmonotonous behavior with λ at $z \geq 2$. Besides, the critical amplitude depends on λ very weakly. As expected, the approximation considered in this work predicts the mean-field critical behavior for size- and charge-asymmetric primitive models in the vicinity of the critical point. A comparison with the available theoretical and simulation results is given.

Interstitial Fe-Cr alloys: Tuning of magnetism by nanoscale structural control and by implantation of nonmagnetic atoms

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Using the density functional theory, we perform a full atomic relaxation of the bulk ferrite with 12.5%-concentration of monoatomic interstitial Cr which is periodically located at the edges of the bcc Fe_α cell. We show that structural relaxation in such computationally engineered alloys leads to significant atomic displacements and results in the formation of novel highly stable configurations with parallel chains of octahedrically arranged Fe. The enhanced magnetic polarization in the low-symmetry metallic state of this type of alloys can be externally controlled by additional inclusion of nonmagnetic impurities like nitrogen. We discuss possible applications of generated interstitial alloys in spintronic devices and propose to consider them as a basis of novel durable types of stainless steels.

Quasistatic heat processes in mesoscopic non-equilibrium systems

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Quasistatic processes play an important role in building up the thermodynamic formalism, both in equilibrium and beyond. A basic difficulty in the non-equilibrium case is the divergence of energy flows between system and its environment in the quasistatic limit. We discuss various approaches how to overcome this problem by constructing finite (excess) parts of these energy flows. It has also been recently proposed that for weakly non-equilibrium processes the excess heat (approximately) satisfies thermodynamic relations extending those for equilibrium processes, with a generalized entropy function. In order to systematically analyze these propositions, we first derive non-perturbative formulas for quasistatic excess path quantities in markovian systems, and we propose a method how to possibly access them experimentally. By extending the method of McLennan, we perturbatively construct the excess work and heat for both over- and under-damped diffusions driven by small non-gradient forces. It is shown that the excess heat always satisfies the (generalized) Clausius relation up to the first order in non-equilibrium driving, whereas this is no longer true in general when beyond the leading order. In the latter case, the excess path quantities do not derive from (generalized) thermodynamic potentials but they require new non-potential corrections, as demonstrated numerically. We also discuss the possible meaning of those new corrections.

Structural and thermodynamical properties of the restricted primitive model electrolyte in a mixture with uncharged hard-spheres. A grand canonical Monte Carlo simulation and HNC integral equation study

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We studied a restricted primitive model electrolyte in a mixture with uncharged hard-spheres using the grand canonical Monte Carlo (GCMC) computer simulation and Ornstein-Zernike integral equation theory in the hypernetted chain approximation. From GCMC we obtained radial pair distribution functions of species of the system, excess internal energy, excess chemical potential, and the heat capacity at constant volume in a wide range of changes of the chemical potential of species. In addition, we have calculated the isothermal compressibility by using integral equations. In majority of cases, we obtained good agreement of the theory with simulations.

Adsorption of a solvent primitive model for electrolyte solutions in disordered porous matrices of charged species. Replica Ornstein-Zernike theory and grand canonical Monte Carlo simulations

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A theoretical study of a quenched–annealed system in which an annealed component is the restricted primitive model electrolyte in a mixture with hard sphere species (SPM) whereas disordered quenched medium is modeled as the restricted primitive model (RPM) electrolyte is presented. The annealed mixture is in thermal and chemical equilibrium with an external reservoir containing the same SPM. The system is studied by using the replica Ornstein–Zernike (ROZ) integral equation theory and grand canonical Monte Carlo simulations. We are primarily interested in collecting computer simualtion data and compare them with theoretical predictions. In terms of physical observables our focus is in the selectivity effects of adsorption of each species of the mixture described by the adsorption isotherms as well as by the composition isotherms. The influence of ionic matrix density and of the bulk state of the mixture on selectivity are examined in detail. Besides, we analyze the dependence of internal energy on the conditions of adsorption and the constant volume heat capacity. Finally, our results concern the activity coefficients of adsorbed species on the applied chemical potentials. In general, the theory we use is in a very good agreement with computer simulations.

Vertex corrections to the electrical conductivity of the Falicov-Kimball model

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We use a systematic expansion around the mean-field solution via the asymptotic limit to high spatial dimensions to study effects of elastic scatterings of mobile electrons on either thermally equilibrated or frozen, randomly distributed static impurities. We concentrate on quantum coherence effects and calculate the leading-order vertex corrections to the mean-field (Drude) electrical conductivity. We demonstrate that the sign of the vertex correction is always negative and the quantum coherence due to elastic backscatterings always leads to diminution of diffusion. The cases of Falicov-Kimball model with symmetric binary disorder and box disorder are studied.

On origin of correlations in infinite-particle Bose and Fermi systems

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We consider the microscopic origin of the rigorous description of non-equilibrium correlations of Bose and Fermi many-particle systems.

Correlation operators that give an alternative description of the quantum state evolution are defined by means of cluster expansions of density operators, which are the solutions of the initial value problem of the von Neumann equations. We deduce the von Neumann hierarchy that governs the evolution of correlation operators and construct the solution of its initial-value problem for the case of a n-body interaction potential. The properties of the group of nonlinear operators generated by the von Neumann hierarchy are examined.

The links of constructed solution of the von Neumann hierarchy both with the solution of the BBGKY hierarchy for marginal density operators and with the nonlinear BBGKY hierarchy for marginal correlation operators are discussed.

Method of calculating the free energy of a 3D Ising-like system taking into account the correction for the interaction potential averaging

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With allowance for the non-Gaussian quartic measure density and the correction for the potential averaging, the calculation of the partition function for a three-dimensional one-component spin system is performed using the collective variables method described in [1,2]. In contrast to our previous studies, the integration over the layers of the phase space of collective variables is carried out considering the dependence of the Fourier transform of the interaction potential on the wave vector. The resulting recurrence relations are written and analyzed. The critical exponents of the correlation function and correlation length as well as the explicit expressions for the free energy and susceptibility of the system are obtained by exploiting a unified approach. The values of the critical exponents of the susceptibility and specific heat, renormalized due to the above-mentioned correction, are estimated.

[1] Yukhnovskii I.R., Phase Transitions of the Second Order. Collective Variables Method. World Scientific, Singapore, 1987.
[2] Yukhnovskii I.R., Kozlovskii M.P., Pylyuk I.V., Microscopic Theory of Phase Transitions in the Three-Dimensional Systems. Eurosvit, Lviv, 2001 (in Ukrainian).

The order parameter and susceptibility of a 3D Ising-like system in an external field

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We consider a $3D$ Ising-like model in the presence of an external field in the vicinity of critical point. The interaction between spins on a simple cubic lattice is presented by exponentially decreasing potential. The method of collective variable is used. The calculations are performed within the framework of "ρ^4-model".

The main results are the explicit analytical expressions obtained for the order parameter and susceptibility of such a system as functions of the reduced temperature $\tau = (T - T_c)/T_c$ (T_c is the critical temperature), the external field h and the microscopic parameters of Hamiltonian [1]. The temperature region from $-\tau^*$ up to τ^*, where $\tau^* = 0.02$, is covered. As well, these quantities are presented in the scaling forms and a comparison with results obtained by others methods is made.

[1] Kozlovskii M.P., Romanik R.V., Condens. Matter Phys., 2010, **13**, 43004.

Phase behavior of heteronuclear rigid trimers

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Monte Carlo simulation within the grand canonical ensemble, the histogram reweighting technique are used to explore the phase behaviour of heteronuclear rigid rods trimers, composed of A and B type segments, on a square lattice. The structural transition between disorder fluid and ordered fluid have been observed. It is shown that the order-disorder phase transition may occur via a continuous as well as first-order phase transition. It is found that the phase diagrams exibit the presence of critical, tricritical, and critical end points, depending on the magnitudes of coupling constans. The critical exponents associated with the continuous phase tyransitions have been estimated using the finite size scaling analysis.

The influence of the barrier transparency on the stationary properties of superconducting junctions of SIS-type

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We investigate theoretically the influence of the barrier transparency on the stationary properties of superconducting junctions of SIS-type. The temperature is assumed to be close to the critical one, because the Ginzburg-Landau theory is used in the work. We have derived the boundary conditions for the Ginzburg-Landau equation, which are valid for arbitrary barrier transparency. To obtain the boundary conditions we consider the space behavior of the order parameter near IS interface within the framework of the microscopic theory of superconductivity and use the so-called method of quasiorthogonality to asymptotics. We analyze the form of the current-phase relation for a number of values of the barrier transparency. For the barrier transparency about $0,5$ critical current in the junction is close to the depairing current in a homogenous superconductor is shown. With barrier transparency increase maximum of the function $I_s(\varphi)$ is shifted into region $\varphi<\pi/2$. We have also obtained the analytical result for $I_s(\varphi)$, which is well coordinated with the numerical one under condition $D \leq 0,5$.

In additional we investigate both the critical current I_c and the critical phase φ_c as function of barrier transparency. The order parameter and the superfluid velocity as function of the distance to the IS-interface is also studied.

Langevin Brownian dynamics simulation of hard spheres

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The blossoming of interest in colloids and nano-particles has given renewed impulse to the study of hard-body systems. In particular, hard spheres have become a real test system for theories and experiments. It is therefore necessary to study the complex dynamics of such systems in presence of a solvent; disregarding hydrodynamic interactions, the simplest model for the dynamics is the Langevin equation. Unfortunately, standard algorithms for the numerical integration of the Langevin equation require that interactions are slowly varying respect to the integration timestep. This in not the case for hard-body systems, where there is no clearcut between the correlation time of the noise and the timescale of the interactions. Starting first from a splitting of the Fokker-Plank operator associated with the Langevin dynamics, and then from an approximation of the two-body Green's function, we introduce and test two new algorithms for the simulation of the Langevin dynamics of hard-spheres.

Lattice dynamics model of hydrogen-bonded crystals of KH_2PO_4-type

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A semi-phenomenological atomistic model of lattice dynamics of hydrogen-bonded dielectric crystals of KH_2PO_4-type is presented. The model takes into account the long-range Coulomb, short-range Born-Mayer-type and covalent interatomic interactions. "Oxygen-hydrogen" interactions within the $O - H(D) \cdots O$ hydrogen bonds were simulated like the weak covalent interactions. The current version of the model operates with seven adjustable parameters.

The lattice dynamics of CsH_2PO_4, CsD_2PO_4, RbD_2PO_4, $PbHPO_4$, $PbDPO_4$, TlH_2PO_4 and TlD_2PO_4 crystals was simulated basing on this atomistic model. The phonon spectrum in Brillouin zone centre, phonon dispersion relations along the symmetric directions in reciprocal space, density of phonon states, partial density of states, dispersion of atomic mean-square displacements and structure factors were calculated in various structure phases of all the crystals mentioned above. The calculation gives rather reasonable agreement with the experimental data. For example, the overall discrepancy between the experiment and our simulation for the fundamental (Γ-point) phonon frequencies does not normally exceed 8 % for the majority of compounds studied within the current approach.

The lattice dynamics simulation enables us to interpret the set of spectroscopic, acoustic and structural experimental data of many hydrogen-bonded crystals of KH_2PO_4-type. Basing on this model we simulated the conditions of some structural phase transitions occurred in these compounds.

Hard convex body fluids in random porous media

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Despite intense investigation of fluid adsorption in random porous media during the last two decades the first analytical results for such confined fluids appeared very recently. In [1] an extension of the scaled particle theory (SPT) capable of describing a hard sphere fluid in hard sphere or overlapping hard sphere matrices was proposed. Later in [2] this approach was improved and an excellent agreement with computer simulations was reached.

In this report we present generalization of the SPT theory for the description of hard convex body fluids in random porous media. As a result, analytical expressions for the chemical potential and the equation of state of hard convex body fluids in hard convex body and overlapping hard convex body matrices are obtained. The influence of non-spherical shapes of fluid molecules and matrix particles on thermodynamic properties is discussed.

[1] M. Holovko, W. Dong, J. Phys. Chem. B, 2009, **113**, 6360.
[2] T. Patsahan, M. Holovko, W. Dong, J. Chem. Phys., 2011, **134**, 074503.

Thermodynamic Casimir effect in isotropic and anisotropic systems

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In 1948, Casimir predicted the existence of an attractive force between two conducting plates resulting due to quantum fluctuations of electromagnetic field in the vacuum. Since that time, investigations of long-range fluctuation-induced forces in constrained systems attracted enormous interest. The Casimir effect has been associated with very different phenomena ranging from sticking of parts in nanoscale devices through the quantum levitation to cosmologic problems and reaching faster-than-light velocities.

The present communication addresses the theoretical treatment of a thermodynamic version of this effect induced by long-range nearly-critical fluctuations, performed in collaboration with M. Burgsmüller, H.W. Diehl, and D. Grüneberg from the Duisburg-Essen University.

In d dimensional slabs of isotropic systems, at bulk critical point the effective forces between boundaries decay as $\propto \Delta L^{-\lambda}$ with $\lambda = d$ for large thickness L. We showed that the usual $\varepsilon = 4 - d$ expansion of universal Casimir amplitudes Δ breaks down beyond first order when periodic or Neumann-Neumann boundary conditions (BC) are applied to the confining surfaces. We explicitly obtained non-analytic corrections $\propto \varepsilon^{3/2}$ preceding the usual $O(\varepsilon^2)$ term and predicted the integer powers of $\ln \varepsilon$ in higher-order contributions.

Strongly anisotropic systems (SAS) exhibit special features. They have (at least) two distinct correlation lengths parallel and perpendicular to the anisotropy axes related via $\xi_\parallel \sim \xi_\perp^\theta$ where the anisotropy index $\theta \neq 1$. Hence in film geometries, boundaries of different orientations with respect to these intrinsic directions produce different effects. The Casimir-like forces behave as $\propto \Delta_{\parallel,\perp} L^{-\lambda_{\parallel,\perp}}$ with different universal amplitudes, decay exponents, and nonuniversal prefactors. For m-axial SAS we found $\lambda_\parallel = d - m + \theta m$ and $\lambda_\perp = (d-m)/\theta + m$. We calculated the amplitudes $\Delta_{\parallel,\perp}$ for anisotropic slabs with periodic and free BC at bulk Lifshitz points in the Gaussian approximation, $\epsilon = 4 + m/2 - d$ expansion, and spherical limit. In two special cases we reproduce the earlier results for smectic liquid crystals in film geometries of different orientations.

Equation of state for extrasolar giant planets

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An equation of state for a mixture of metallic hydrogen and atomic helium has been proposed. The explored intervals of pressure, temperature, and density correspond to the conditions on the largest solar system planets, Jupiter, Saturn and several dozen of extrasolar planets. The substance of a planet is modelled as a mixture of protons, helium atoms, and electrons. A theory, where the electron-proton and electron-atom interactions are considered as a perturbation, has been used to find the pressure in the mixture. The electron subsystem is analyzed in the random phase approximation, and the proton-proton, atom-atom, and proton-atom interactions in the hard-sphere approximation. The applicability of the polytropic sphere model for the simulation of Jupiter's and Saturn's internal structures has been analyzed, and a specific value for the polytropic index has been proposed. The density, pressure, and temperature on Jupiter and Saturn as functions of the distance from the planet center have been found. Possible fractions of hydrogen and helium in the planet composition have been estimated

Thermodynamic metallization parameters of helium

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By now helium is still not obtained in a metallic state. Still unknown even values of its thermodynamic parameters at the point of metal-insulator transition. In this paper we determined the density and temperature of helium in that point. We calculated the pressure and electrical resistivity of metallic helium in a wide range of temperatures and densities. For the helium in the metal state used the two-component almost free electrons model. We believed that the system consists of only single ionized helium ions and conduction electrons. Electron-electron interaction was accounted for diffraction model of a metal. To describe electron-ion interaction used the exact electrostatic potential generated helium ions. For the ion subsystem used model of hard spheres. The hard spheres diameter was determined in two ways: from analysis of effective pair interactions between the ions and with help of variational method from the minimum free energy of liquid helium at the given temperature and density. Both methods give similar results. Density of helium at the point of metal-insulator transition was found from the divergence condition in the perturbation series for electrical resistivity of metal helium. It turned out to equal 3.8 g/cm3. Transition temperature determined from the analysis of the depth of potential well for the pair effective ion-ion interaction. She proved equal to 12000–160000 K. The pressure in the vicinity of the phase transition point was obtained with the help of microscopic equation of state in the second order perturbation theory for electron-ion interaction. He was equal 1.6–2.0 Mbar. To find the electrical resistivity was used the perturbation series for electron-ion interaction, because when approaching a phase transition point the role of members of the old order quickly growing. As the density of helium at the point of transition is used its value when the electrical resistivity reached a critical value for metal – 500 $\mu\Omega$ cm

Sounds in the dilute condensed Bose-gas

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We study the propagation of sound waves in a trapped dilute condensed Bose-gas at finite temperatures. The dispersion law for sound waves in terms of the equations of a condensed Bose-gas dynamics at finite temperatures has been obtained. These equations are the Gross-Pitaevskii equation for condensate that was generalized for the finite temperatures case and the quantum Boltzmann kinetic equation for the noncondensate (thermal cloud). We have used modified Wang Chan method to derive the dispersion law for sound waves, in which solution of the linearized Boltzmann kinetic equation can be found in form of the plane wave.

Variational approach to the spectra of sparse random matrices

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We show by direct calculation that the replica and cavity methods are exactly equivalent for the spectrum of Erdős-Rényi random graph. We introduce a variational formulation based on the cavity method and use it to find approximate solutions for the density of eigenvalues. We also use this variational method for calculating spectra of sparse covariance matrices.

Two approaches to description of fractional Brownian motion

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In this contribution we consider two natural approaches to studying fractional Brownian motion (fBm). The first one is based on the generalized Fokker-Planck equation. We suggest a consistent mathematical approach to the derivation of the latter and show several examples of how the developed technique may be applied, including the calculation of the thermodynamic work probability density function (PDF), and the PDF for the fBm in the linear oscillator's field. With the help of the second approach which involves numerical simulations of the overdamped Langevin equation with fractional Gaussian source, we study the Kramer's problem for fractional Brownian motion, that is the escape from a potential well, underlining both remarkable differences and similarities with the classical Brownian motion case.

Propagation of relativistic charged particles in ultracold atomic gases with Bose-Einstein condensates

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We consider some effects arising at charged particle propagation in Bose-Einstein condensate (BEC) of alkali metals atomic gasses. The charged particle energy change in Vavilov-Cherenkov phenomenon in a gas with condensate is studied. It is shown that to gain Cherenkov effect in the investigated system the particles must have high (relativistic) velocity since in rarified gasses refractive index is close to unity in resonant frequencies range. The particles energy change while propagating through BEC are defined via gas permittivity expressions. It is shown that the particle under certain conditions is capable of both loosing the energy and acceleration by the ultracold gas. The basic case of relativistic particle acceleration by a rarified gas of atoms at temperatures close to absolute zero is discussed. The possibilities of atomic spectral characteristics definition with help of Cherenkov effect in gas with BEC are studied. It is shown that by means of particle velocity variation and thus, the definition of gas refractive index maximum, we can determine natural atomic spectral level width if we know additional spectral or microscopic characteristics of atoms.

Hydrodynamics of two-component liquids taking into account relaxation phenomena

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We discuss dynamics of two-component system described by the Landau kinetic equation for distribution functions $f_{ap}(x,t)$ $(a=1,2)$. The consideration is based on the Chapman-Enskog method generalized with the Bogolyubov idea of the functional hypothesis. According this idea (see, for example, [1]) after some time τ_0 distribution functions $f_{ap}(x,t)$ have the structure $f_{ap}(x,\xi(t))$ where $\xi_\mu(x,t): n_1(x,t), n_2(x,t), v_l(x,t), T(x,t), u_l(x,t), \tau(x,t)$ are usual hydrodynamic variables and additional values $u_l(x,t), \tau(x,t)$ which give velocities $v_{al}(x,t)$ and temperatures $T_a(x,t)$ of the components

$$v_{1l}=v_l+u_l, \quad T_1=T+\tau, \quad v_{2l}=v_l-\frac{m_1n_1}{m_2n_2}u_l, \quad T_2=T-\frac{n_1}{n_2}\tau.$$

These variables are defined by standard expressions

$$\int d^3p f_{ap}(x,\xi)=n_a(x), \qquad \int d^3p p_l f_{ap}(x,\xi)=m_a n_a(x) v_{al}(x),$$

$$\int d^3p \frac{(p-m_a v_a)^2}{2m_a} f_{ap}(x,\xi)=\frac{3}{2}n_a(x)T_a(x).$$

We study states of the system which are close to usual hydrodynamic states considering values $u_l(x,t), \tau(x,t)$ as a small ones of the same order λ $(\lambda \ll 1)$. Gradients of all introduced variables are assumed to be of the order g $(g \ll 1)$ where values λ and g are independent. It has been shown that in the considered theory the leading contributions to distribution functions $f_{ap}(x,\xi)$ are not given by the Maxwell distribution

$$w_{ap}(n_a,T_a,v_a)=\frac{n_a}{(2\pi m_a T_a)^{3/2}}\exp\left\{-\frac{(p-m_a v_a)^2}{2m_a T_a}\right\}$$

and usual local equilibrium assumption is not valid.

[1] A.I. Akhiezer, S.V. Peletminsky. Methods of Statistical Physics. London, Pergamon Press, 1981.

To phonon hydrodynamics in crystalline solid

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It is assumed that crystal has one particle in a cell of the lattice. Therefore, nonequilibrium states of acoustic phonons are discussed. Dynamics of this system is described by kinetic equation for phonon distribution function $f_{\alpha p}(x,t)$. Consideration is based on the Chapman-Enskog method modified according to the Bogolyubov idea of the functional hypothesis. In this approach (see, for example, [1]) distribution function is a functional $f_{\alpha p}(x,\xi(t))$ of phonon subsystem temperature $\xi_0(x,t) = T(x,t)$ and drift velocity $\xi_n(x,t) = u_n(x,t)$. Here we use standard definitions of these values

$$\sum\nolimits_{\alpha} \int d^3p\, f_{\alpha p}(x,\xi)\zeta_{\mu\alpha p} = \sum\nolimits_{\alpha} \int d^3p n_{\alpha p}(\xi(x))\zeta_{\mu\alpha p},$$

where $n_{\alpha p}(\xi) \equiv [\exp\beta(\varepsilon_{\alpha p} - p_n u_n) - 1]^{-1}$ (the Planck distribution) is equilibrium distribution for phonon gas moving with the velocity u_n ($\zeta_{0\alpha p} \equiv \varepsilon_{\alpha p}, \zeta_{n\alpha p} \equiv p_n$ are energy and momentum of a phonon; $\beta \equiv 1/T$; $\mu = 0, n$).

Phonon hydrodynamics is built for crystal of the cubic system (classes O, O_h, T_h) for a case of small velocity $u_n(x,t)$. It has been shown that the Planck distribution with velocity $n_{\alpha p}(\xi(x,t))$ does not give leading contribution to phonon distribution function $f_{\alpha p}(x,\xi(t))$. So, the local equilibrium assumption is not valid for phonon hydrodynamics. However, standard approach to phonon hydrodynamics is based on this idea (see review [2]).

[1] A.I. Akhiezer, S.V. Peletminsky. Methods of Statistical Physics. London, Pergamon Press, 1981.
[2] A.I. Akhiezer, V.F. Aleksin, V.D. Khodusov, Low temperature physics, 1994, **20**, No.12, 1199 (in Russian).

Density functional theory of adsorption on surfaces modified with tethered brushes

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A density functional approach to adsorption and phase behavior of a simple fluid from gas phase on a surface modified with a small amount of grafted chains is presented. The chains are modeled as freely jointed tangent spheres with end segments attached to the surface. The segments and gas molecules interact via the Lennard-Jones potential. We have found that the presence of preadsorbed chains considerably affects wettability of solid surfaces. An increase in the amount of grafted chains leads to a crossover between prewetting and layering transitions. This crossover occurs by merging of successive layering transitions. In order to illustrate those phenomena, phase diagrams in the chemical potential-temperature and excess adsorption-temperature for selected model systems are presented.

Longitudinal dielectric, piezoelectric and elastic properties of the $K_{1-x}(NH_4)_xH_2PO_4$ type mixed crystals. Simple model

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Within the framework of the simple model for the $K_{1-x}(NH_4)_xH_2PO_4$ type mixed crystals with taking into account random short-range and long-range interactions and the piezoelectric interaction with the shear strain ε_6 in the two-particle cluster approximation we calculate the thermodynamic potentials of the system. Using the appropriate equations of state, we calculate x-T phase diagram, spontaneous polarization, longitudinal dielectric permittivity of mechanically free and clamped crystals, their piezoelectric characteristics, elastic constants and molar specific heat.

[1] Levitsky R.R., Zachek I.R., Vdovych A.S., Journal of National University "Lvivska Politechnika", Phys. and math. sciences, 2009, **660**, No 660, 80 (in Ukrainian).
[2] Sorokov S.I., Levitskii R.R., Vdovych A.S., Condens. Matter Phys., 2005, **8**, No 3(43), 603.
[3] Sorokov S.I., Vdovych A.S., Levitskii R.R., J. Phys. study., 2009, **13**, No 1, 1701 (in Ukrainian).

Dielectric and superfluid-like states of one-dimensional ionic Pauli conductor

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We focus on the features of spectra and diagrams of states obtained via exact diagonalization technique for finite ionic conductor chain in periodic boundary conditions. One-dimensional ionic conductor is described with the lattice model where ions are treated in frames of 'mixed' Pauli statistics. The ion transfer and nearest-neighbour repulsive interaction between ions are taken into account. The spectral densities and diagrams of states for various temperatures and strength of interaction are obtained. The conditions of transition from uniform (Mott insulator) to the modulated (charge density wave state) through the superfluid-like state (similar to state with the Bose-Einstein condensate observed in hard-core boson models) are analyzed.

Dynamic properties of quasi-one-dimensional structures with hydrogen bonds

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The dynamical conductivity of the quasi-one-dimensional structures with hydrogen bonds is studies on the bases of proposed pseudospin-electron model. It is taken into account the proton-electron interaction, external longitudinal field, the tunneling hopping of protons, electron transfer and direct interaction between protons. The proton subsystem is described by the pseudospin formalism.

The dependence of the electron concentration and mean number of protons on site on temperature and external field are obtained. It was shown that abrupt changes of these characteristics at the first-order phase transition is smaller for the structures with a high proton tunneling frequency and stronger direct interaction between protons. The phase transition lines from uniform phase into charge ordered phase is determined. The dependence of the dynamical conductivity on temperature and external field and it changes at the phase transitions are obtained.

Thermodynamic properties of the spin-1/2 Ising-Heisenberg model on a triangle-hexagon lattice

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Thermodynamic properties of a geometrically frustrated spin-1/2 Ising-Heisenberg model on a triangle-hexagon lattice are investigated within the framework of an exact analytical approach based on the generalized star-triangle mapping transformation. With the help of this method, exact analytical results for the free and internal energy, spontaneous magnetization and specific heat are derived from a precise mapping equivalence with the corresponding quantities of the spin-1/2 Ising model on a triangular lattice. Apart from the classical ferromagnetic phase with a perfect alignment of all the Ising as well as Heisenberg spins, the spin-1/2 Ising-Heisenberg model with the ferromagnetic Heisenberg interaction may also display an unusual spontaneously long-range ordered phase with the obvious quantum reduction of the spontaneous magnetization. It is found that this striking spontaneously long-range ordered phase emerges owing to a mutual interplay between the easy-axis Ising interaction and the easy-plane Heisenberg interaction. In addition, the disordered spin-liquid phase with a non-zero residual entropy may constitute the ground state even if all the considered interactions are assumed to be ferromagnetic. It is evidenced that the specific heat may exhibit interesting thermal dependencies either with a pronounced logarithmic singularity accompanied with an additional round maximum or with two round maxima well separated one from the other.

Hydrodynamic modes in external fluctuating field

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Hydrodynamics of the liquid charged dielectric with constant dielectric permittivity in external potential electric field or neutral gas in the same gravitation field is studied. The field is characterized by the second correlation moment of strength $\vec{E}$. Motion of environment is described by the charge conservation law $\partial_t\rho + \mathrm{div}\rho\vec{v} = 0$, mass one $\partial_t\sigma + \mathrm{div}\sigma\vec{v} = 0$, which is a charge in case of gravitation interaction, and Euler equation, which for definiteness we write down for dielectric in electric field $d\sigma\vec{v}/dt = -\nabla P + \rho\vec{E}$. Generated by own motion selfconsistent field appears here besides external one. This field is determined by Poisson $\mathrm{div}\varepsilon\vec{E} = 4\pi\rho$ and Maxwell equations [1] $\partial\varepsilon\vec{E}/\partial t = -4\pi(\rho\vec{v})^{\|}$, where it is taken into account, that $\mathrm{rot}\vec{E} = 0$. Then it is possible to rewrite $\rho E_\alpha = \left\{\nabla_\beta\varepsilon E_\beta E_\alpha - \nabla_\alpha\varepsilon E^2/2\right\}/4\pi$. We average on the accidental phase of the fluctuating field. And we consider small amplitudes. $\sigma_0\partial v_\alpha/\partial t = -\nabla_\alpha P + \rho_0 E_\alpha + \rho E_{\alpha 0} + \varepsilon\left\{\nabla_\beta\overline{E_\beta E_\alpha} - \nabla_\alpha\overline{E^2}/2\right\}/4\pi$. A new variable is entered in this equation - centered correlation of the electric field $\overline{E_\beta E_\alpha}$, for which we receives temporal equation, using Maxwell equation with current in hydrodynamic approximation. We assume that the centered correlation of external field is isotropic but nonhomogeneous set value $\overline{E_\beta E_\alpha}(r) = \delta_{\alpha\beta}\overline{E^2}(r)/3 + E_{\alpha 0}E_{\beta 0}$, then $\partial\overline{E_\gamma E_\alpha}/\partial t = \vec{v}_\gamma^{\|}\nabla_\alpha\overline{E^2}(r)/6 + \vec{v}_\alpha^{\|}\nabla_\gamma\overline{E^2}(r)/6$. And we consider long waves. Characteristic equation gives Langmuir frequencies $\omega^2 = 4\pi\rho_0^2/\varepsilon\sigma_0 - \varepsilon\Delta\overline{E^2}(r)/24\pi\sigma_0$ with correction from field correlation. For the case of gravitation field it is simply necessary to replace in all formulas $\varepsilon \to -1/G$ and $\rho \to \sigma$. And we obtain corrected Jeans frequency.

[1] A.A. Stupka, Journal of Astrophysics and Astronomy, 2008, **29**, No 3-4, 379.

Steady state traffic flow on a multilane road

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Statistical mechanics of a system of many types of cars on a multilane road is developed. Behaviour of cars is defined by a conditional probability of car velocity depending on the distance and velocity of the car ahead and in the next lane. A system consisting of different cars is modelled by a system of many types of cars differing in maximal velocity and efficiency of brakes. Starting from conditional probabilities and using principle of maximum entropy, probability densities of car velocities, headways anf traffic flow are calculated. It is shown that the first-order phase transition between free flow and congested traffic may be driven by number of fast cars in a system of slow cars, and, as a rule, admixture of cars of superior qualities does not increase but decreases the total flow. In the system of cars with poor brakes, platoons of cars of the same velocity are formed. The effect of number of parallel lanes on total traffic flow is shown.

Application of principle of maximum entropy was justified by comparing the results with steady state properties of exactly solvable disordered simple kinetic models and an equivalent, numerically solved, kinetic model.

Generalized elastic models: fractional dynamics representation and beyond

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The Generalized Elastic Model accounts for the dynamics of several physical systems, such as polymers, fluctuating interfaces, growing surfaces, membranes, proteins and file systems among others. We derive the fractional stochastic equation governing the motion of a probe particle (tracer) in such kind of systems. This Langevin equation involves the use of fractional derivative in time and satisfies the Fluctuation-Dissipation relation, it goes under the name of Fractional Langevin Equation. Within this framework the spatial correlations appearing in the Generalized Elastic Model are translated into time correlations described by the fractional derivative together with the space-time correlations of the fractional Gaussian noise. We derive the exact scaling analytical form of several physical observables such as structure factors, roughness and mean square displacement. Special attention will be devoted to the dependence on initial conditions, linear-response relations in the case of an applied potential and non-linear interactions.

[1] Taloni A., Chechkin A., Klafter J., Phys. Rev. Lett., 2010, **104**, 160602.
[2] Taloni A., Chechkin A., Klafter J., Phys. Rev. E, 2010, **82**, 061104.

Nonequilibrium statistical operator method in Renyi statistics

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The generalization of the Zubarev nonequilibrium statistical operator method for the case of Renyi statistics is proposed when the relevant statistical operator (or distribution function) is obtained based on the maximum entropy principle for the Renyi entropy. The nonequilibrium statistical operator and corresponding generalized transport equations for the parameters of the reduced description are obtained with regard to Kawasaki-Gunton and Mori projection.

Such an approach is applied to a consistent description of kinetic and hydrodynamic processes in the system of classical interacting particles. As a result both the nonequilibrium statistical operator and the generalized transport equations are obtained, when the nonequilibrium one-particle distribution function $f_1(x;t) = \langle \hat{n}_1(x) \rangle^t$ along with the nonequilibrium averaged value of the potential energy of interaction $\langle \hat{\varepsilon}_{int}(\vec{r}) \rangle^t$ are selected as the reduced-description parameters. At the Renyi parameter $q = 1$ the known results based on the Gibbs statistics are reproduced.

[1] B.B. Markiv, R.M. Tokarchuk, P.P. Kostrobij, M.V. Tokarchuk, Physica A, 2011, **390**, 785.

Magnetocaloric effect and magnetic cooling in the spin-$\frac{1}{2}$ XX chain with three-site interactions

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The magnetocaloric effect is the temperature change of a magnetic system under an adiabatic variation of the external magnetic field, i.e., $(\partial T/\partial H)_S = -(T/C_H)(\partial S/\partial H)_T$. The magnetocaloric effect in quantum spin chains has been a subject of many studies in recent years [1–3].

In our work we examine the magnetocaloric effect in the spin-$\frac{1}{2}$ XX chain with three-site interactions with the Hamiltonian [4,5]

$$\mathcal{H} = \sum_n \left[-h s_n^z + J\left(s_n^x s_{n+1}^x + s_n^y s_{n+1}^y\right) + K\left(s_n^x s_{n+1}^z s_{n+2}^x + s_n^y s_{n+1}^z s_{n+2}^y\right) \right.$$
$$\left. + E\left(s_n^x s_{n+1}^z s_{n+2}^y - s_n^y s_{n+1}^z s_{n+2}^x\right) \right] .$$

Here h is the external magnetic field, J is the XX interaction constant, and K and E are the constants of three-site interactions of $XZX+YZY$ and $XZY-YZX$ types, respectively. The spin model can be mapped onto a free-fermion system via the Jordan-Wigner transformation. Rigorous analysis shows that it exhibits a rich ground-state phase diagram.

We calculate the entropy per site $s(T,h)$ of the spin model to discuss *(i)* how the adiabatic change of magnetic field h influences the temperature T of the spin system in the presence of the three-site interactions and *(ii)* how the isothermal change of magnetic field h influences the entropy s of the spin system in the presence of the three-site interactions. We find that the quantum phase transition lines clearly manifest themselves for the magnetocaloric effect in the small-s or small-T regimes.

[1] Zhitomirsky M.E., Honecker A., J. Stat. Mech.: Theory Exp., 2004, P07012.
[2] Honecker A., Wessel S., Condens. Matter Phys., 2009, **12**, 399.
[3] Wolf B. et al. Preprint arXiv:1012.3328.
[4] Titvinidze I., Japaridze G.I., Eur. Phys. J. B, 2003, **32**, 383.
[5] Lou P., Wu W.-C., Chang M.-C., Phys. Rev. B, 2004, **70**, 064405.

Many-fermion dynamic structure factors for the spin-$\frac{1}{2}$ XX chain with three-site interactions of $XZY - YZX$ type

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We consider the spin-$\frac{1}{2}$ XX chain in a transverse magnetic field with three-site interactions of $XZY - YZX$ type which is governed by the Hamiltonian

$$H = \sum_n \left[J \left(s_n^x s_{n+1}^x + s_n^y s_{n+1}^y \right) - h s_n^z + E \left(s_n^x s_{n+1}^z s_{n+2}^y - s_n^y s_{n+1}^z s_{n+2}^x \right) \right]$$

to discuss dynamic properties of the model. The considered spin model is exactly solvable since it can be reduced to free fermions after exploiting the famous Jordan-Wigner transformation.

In our previous study [1] we discussed two-fermion dynamic structure factors, like $S_{zz}(\kappa, \omega)$, which can be calculated analytically and therefore can be studied in great detail. In the present study we focus on many-fermion dynamic structure factors, like

$$S_{xx}(\kappa, \omega) = \sum_m e^{-\mathrm{i}\kappa m} \int_{-\infty}^{\infty} \mathrm{d}t e^{\mathrm{i}\omega t} \langle s_n^x(t) s_{n+m}^x \rangle.$$

Theses quantities can be calculated analytically only in the high-temperature limit $T \to \infty$ or in the strong-field regime at $T = 0$. For arbitrary values of the temperature and Hamiltonian parameters many-fermion dynamic structure factors can be computed numerically [2] for chains of several hundred of sites. We compare the obtained numerically xx dynamic structure factor with exact analytical results available in the limiting cases as well as with the zz dynamic structure factor [1]. We demonstrate that the two-fermion excitations which exclusively determine $S_{zz}(\kappa, \omega)$ may be also important for $S_{xx}(\kappa, \omega)$, however, only in the limit $T \to 0$. With temperature increase many-fermion excitations come into being and drastically change $S_{xx}(\kappa, \omega)$.

[1] M. Topilko, O. Derzhko, T. Krokhmalskii, Acta Physica Polonica A (accepted); Preprint ICMP-10-07E.
[2] O. Derzhko, T. Krokhmalskii, Phys. Rev. B, 1997, **56**, 11659.

Relaxed optics: present and future

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Relaxed Optics (RO) is the chapter of modern physics of irreversible interactions light and matter [1,2]. It is based on the phenomenological kinetic classification of proper phenomena.

Basic effects of RO are caused of the processes of saturation of excitation of proper centers of the absorption of an irradiation. The model of cascade step-by-step excitation of these centers is represented and discussed. These effects may be have long-range and short-range action nature. First effects are caused phase transformations of "classical" types (thermal and plasmic); second - of "quantum" types (photokinetic).

A usage of this model is illustrated on the examples of the irreversible interaction of laser radiation with indium antimonide (two-dimensional lattice of sphalerite [2]) and silicon (phase diagram [3]). Two regimes of light scattering: on stable and unstable centers, are analyzed too.

This theory allow to explain the chain of possible phase transformations in laser-irradiated materials, including laser generation [1,2], transitions between various crystal phases [3], a chaotization of laser radiation [4], a creation of nanostructures [2], a destruction [1] and other.

Possible ways of the development of RO and a creation of new methods of this science are discussed too.

[1] Trokhimchuck P.P. Foundation of Relaxed Optics. Vezha, Lutsk, 2006.
[2] Trokhimchuck P.P. Mathematical Foundations of the Knowledge. Polymetrical Doctrine. Vezha, Lutsk, 2009 (In Ukrainian).
[3] Philips J.C., Journal of Applied Physics, 1981, **52**, 7397.
[4] Haken H. Laser light dynamics (Vol. 2). North Holland, Amsterdam, 1986.

On the novel concept to an augmented van der Waals theory of the vapor-liquid equilibria

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The genius of van der Waals was to recognize the essential role of excluded volume that together with cohesion are responsible for the existence of a vapor-liquid equlibria in fluids by means of celebrated van der Waals (vdW) equation of state. The commonly used nowdays augmented van der Waals approach is based on the hard-sphere (HS) model to evaluate the excluded volume contribution to system properties. Nonetheless on evident quantitative improvement comparing to the original vdW approach, the vdW/HS approach still suffers from limitation to ambient and not too much elevated temperature range only. As an attempt to remove this drawback we have recently formulated an augmented vdW approach based on the short-ranged attractive interaction in a form of Yukawa (Y) potential.

The methodology of the vdW/Y approach will be formulated and then its implementation for the two most important simple fluids models, namely, the Sutherland and Lennard-Jones, will be presented. The results clearly show that proposed approach may provide a simple and yet quite accurate equations in an analytic form able to perform over all range of thermodynamic conditions.

Generalized quantum kinetic equation for interacting particles with quantum statistics

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Nowadays the considerable progress in the rigorous derivation of quantum kinetic equations in suitable scaling limits is observed. We develop a new formalism for the description of the quantum kinetic evolution based on usage of a non-perturbative solution of the quantum BBGKY hierarchy.

We establish that in case of initial data, which is completely determined by a one-particle density operator, all possible states of infinitely many bosons or fermions at arbitrary moment of time can be described without any approximations by means of a one-particle density operator together with explicitly defined marginal functionals of this one-particle density operator. For this purpose we develop the method of the kinetic cluster expansions of cumulants of scattering operators, which define the evolution operators of every term of expansions of the marginal functionals of the state over the products of a one-particle density operator, and derive the generalized quantum kinetic equation. Thus, for initial states of many-particle systems obeying Fermi-Dirac or Bose-Einstein statistics, which are given in terms of a one-particle marginal density trace-class operator, the equivalence of the Cauchy problem of the quantum BBGKY hierarchy and the Cauchy problem of the generalized quantum kinetic equation is proved.

The specific quantum kinetic equations can be derived from constructed generalized quantum kinetic equation in the appropriate scaling limits or as a result of certain approximations. For example, in the mean-field scaling limit we derive the quantum Vlasov kinetic equation for bosons or fermions. In particular case of pure states it reduces to the nonlinear Schrödinger equation.

[1] Gerasimenko V.I., Tsvir Zh.A., J. Phys. A: Math. Theor., 2010, **43** (48), 485203.
[2] Gerasimenko V.I., Tsvir Zh.A., Math. Bulletin Shevchenko Sci. Soc., 2010, **7**.

Universal amplitude in density-force relations for polymer chains in confined geometries

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The universal amplitude $B_{real} \approx 1.62$ in density-force relations was obtained using the massive field theory approach in fixed space dimensions $d = 3$ up to one-loop order. The obtained universal amplitude is slightly smaller than the previous result of ϵ-expansion $B^{\epsilon}_{real} \approx 1.85$ obtained by Eisenriegler [1] and is in agreement with the MC result $B_{real} \approx 1.70 \pm 0.08$ obtained in Ref. [2] and with result of rough linea extrapolation $B_{extr} \sim 1.4$ obtained on the basis of plotting B_{eff} versus $1/\sqrt{L}$ in Ref.[3]. The knowledge of the universal amplitude B allowed to obtain the layer monomer density profiles for whole class of different systems: 1) a single polymer chain with one end (or both ends) fixed in the half space bounded by the wall; 2) a single chain trapped in the slit of two walls; 3) for the case of dilute and semi-dilute solution of free polymer chains in a half space; 4) for the case of polymer chain in a half space containing a mesoscopic spherical particle of a big radius.

[1] E. Eisenriegler, Phys. Rev. E, 1997, **55**, 3116.
[2] H.-P. Hsu and P. Grasberger, J. Chem. Phys., 2004, **120**, 2034.
[3] A. Milchev and K. Binder, Eur. Phys. J. B, 1998, **3**, 477.

Time dependent spread of a generic 1D wavepacket

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In several problems concerning 1D dynamics, e.g., quantum-state transmission [1], one is faced with the dispersive evolution of an input wavepacket, whose Fourier-space components are determined by its initial shape. The evolution occurs along a 'wire' and is substantially ruled by its dispersion relation ω_k, which is usually a nonlinear function of k when the wire is realized by discrete arrays of physical objects. It is textbook knowledge that a Gaussian packet whose Fourier density is peaked at k_0 travels at the group velocity $v = \omega'_{k_0}$ and its variance broadens according to $\sigma^2(t) = \sigma_0^2 + (\omega''_{k_0}/2\sigma_0)^2\, t^2$, as it happens for the wavefunction of a Schrödinger particle in 1D. However, this case is rather peculiar since its $\omega_k \propto k^2$ has no inflection points.

In order to preserve as much as possible the wavepacket shape one must avoid dispersion: it is therefore convenient to initialize the wavepacket such as k_0 sits on an inflection point of the dispersion relation, i.e., $\omega''_{k_0} = 0$, so that higher-order terms determine the dispersion. In Ref. [2] the role of the cubic nonlinearity of ω_k is accounted for in the case of a Gaussian packet. However, there are reasons to look for an extension of this result: besides the possibility that cubic terms could also vanish (e.g., by symmetry), one could be interested in a non-Gaussian initial shape of the wavepacket. In this work such an extension is obtained in terms of rather simple formulas. These permit to obtain an optimal initial width, which shows peculiar scaling as a function of the wire length.

[1] T.J. Osborne and N. Linden, Phys. Rev. A, 2004, **69**, 052315.
[2] M. Miyagi and S. Nishida, Appl. Opt., 1979, **18**, 678 and 2237.

Nonequilibrium statistical hydrodynamics of ionic systems with taking into account polarization processes

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Statistical description of hydrodynamical processes for ionic molten is proposed with taking into account processes of polarization, caused by deformations of extrinsic ionic shells. This description is obtained with D. Zubarev' method of nonequilibrium statistical operator, appropriate for investigations of both strongly and weakly nonequilibrium processes. The nonequilibrium statistical operator and generalized hydrodynamical equations that take into account polarization processes are received for ionic-polarization model of ionic molten salts, when the observed values (nonequilibrium mean values of ions number, their momentum, dipoles momentum and full energy) are chosen for the shorted description parameters.

Statistical description of electrodiffusion processes in the electron subsystem of a semibounded metal within the generalized jellium model

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Based on the calculation of the quasiequilibrium statistical sum by means of the functional integration method, we obtained a nonequilibrium statistical operator for the electron subsystem of a semibounded metal in the framework of the generalized jellium model in the Gaussian and higher approximations with respect to the dynamic electron correlations. This approach allows one to go beyond the linear approximation with respect to the gradient of the electrochemical potential corresponding to weakly nonequilibrium processes and to obtain generalized transport equations that describe nonlinear processes.

The two-component BCSOS model of surface as a dimerized quantum spin-1/2 chain

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The body-centered solid-on-solid (BCSOS) model of the surface of the two-component crystal is considered. The thermodynamics of the model can be calculated using the transfer-matrix formalism. The transfer-matrix in terms of spin-1/2 operators is found exactly. At low temperatures the problem of finding the thermodynamic properties of the surface is reformulated as the ground-state problem of the one-dimensional dimerized quantum spin-1/2 XXZ model. The latter is considered in the framework of several approximative schemes. On the basis of the ground-state phase diagram of the dimerized quantum spin-1/2 XXZ chain, the temperature phase diagram of the initial surface model is obtained. The relations between the ground-state phases of the quantum chain and the surface phases are also inspected.

Star copolymers in porous environments: scaling and its manifestations

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We consider star polymers, consisting of two different polymer species, in a solvent in the presence of correlated quenched structural obstacles. We assume that the disorder is correlated with a power-law decay of the pair correlation function $g(x) \sim x^{-a}$. In the frames of the field-theoretical renormalization group approach, we analyze different scenarios of scaling behavior working to first order of a double $\varepsilon = 4-d$, $\delta = 4-a$ expansion. We discuss the resulting scaling laws and their possible manifestations in diffusion controlled reactions in the vicinity of absorbing traps placed on polymers in a porous environment as well as the effective short-distance interaction between star copolymers in disordered environment.

[1] V. Blavatska, C. von Ferber, Yu. Holovatch, Phys. Rev. E, 2011, **83**, 011803.

Theoretical prediction and experimental evidence of Blume-Emery-Griffiths phase diagram in the uniaxial $Sn_2P_2S_6$ ferroelectrics

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It has been shown recently [1] that ferroelectric instability in the uniaxial proper ferroelectrics $Sn_2P_2S_6$ (SPS) is driven by non-linear interaction of the low-energy polar B_u mode with the low-energy quadrupole-like full-symmetry mode A_g. The relaxation of a lone-pair located on Sn^{2+} cations leads to the potential energy surface with three wells, which can be described by spin-1 Ising model [2]. It is known [3] that this model represents a large variety of stable, unstable, and metastable phases at different temperatures, and the corresponding phase diagrams contain different kinds of multi-critical points. We derived an effective Hamiltonian, which contains relevant degrees of freedom to describe lattice instability in SPS and defined the unknown parameters from *ab initio* density-functional calculations. We used Metropolis Monte Carlo method to solve the Hamiltonian at different temperatures and pressures. We obtained P-T phase diagram of SPS, which contains pressure induced chaotic phases and phases with quadrupolar ordering in addition to usual para- and ferroelectric phases. Consequent neutron diffuse scattering experiments confirmed the existence of pressure-induced Griffith-like chaotic phase at the pressure of about 0.6 PGa. Work was partially supported by HGF Nachwuchsgruppe Programme VH-NG-409 and Alexander von Humboldt foundation.

[1] K.R. Rushchanskii et al., Phys. Rev. Lett. 2007, **99**, 207601.
[2] M. Blume et al., Phys. Rev. A, 1971, **4**, 1071.
[3] W. Hoston and A.N. Berker, Phys. Rev. Lett., 1991, **67**, 1027.

Latent heat of a traffic model

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We have studied the optimal velocity model [1,2] for highway traffic. On a microscopic level, traffic flow is described by Bando's optimal velocity model in terms of accelerating and decelerating forces. We define an intrinsic energy of the model. We find a latent heat as the system undergoes a phase transition from single phase traffic (free flow) to a phase that contains two different, a dense and a dilute phase (congested or stop–and–go flow). We report on properties of the latent heat.

[1] M. Bando *et al.*, Japan J. Indust. and Appl. Math., 1994, **11**, 203; Phys. Rev. E, 1995, **51**, 1035.
[2] M. Bando *et al.*, J. Phys. I France, 1995, **5**, 1389.

Lattice model of liquid crystalline structures with spontaneously broken chiral symmetry

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By molecular modeling we demonstrate that the nematic long-range order discovered in bent-core liquid-crystal systems should reveal further spatially homogeneous phases. Two of them are identified as a tetrahedratic nematic (N_T) phase with D_{2d} symmetry and a chiral tetrahedratic nematic (N_T^*)phase with D_2 symmetry. These phases were found for a lattice model with quadrupolar and octupolar anisotropic interactions using mean-field theory and Monte Carlo simulations.

Use methods of statistical physics in optimization problems

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Methods of statistical physics were quite effective in applied optimization problems. For optimization problems that contain a large number of variables and parameters, the classical optimization methods were inapplicable. In the optimization problem one can construct an analogue of the Hamiltonian and reduce it to study of the partition function (free energy) of a system. In most cases, the calculation of the partition function can be realized only approximately. One such approximate method is the variational method, which is based on an inequality for the free energy of the system. In most problems the variational inequality is used in the canonical ensemble. However, in a number of problems (depending on the structure of the Hamiltonian) is more convenient to use a variational inequality for the grand partition function. This approach was used particularly in the problem of optimization of the minority game model. An application of variational inequality provides an determination of a trial Hamiltonian. There is a certain arbitrariness in choosing of a trial Hamiltonian, which provides a considerable flexibility to variational method. In the paper in the method of grand partition function the calculations were performed for different trial Hamiltonians. Indicated calculation scheme was used in the minimization problem in one of the Hopfield models. The Hamiltonian of the Hopfield model can be considered as a discrete analogue of the minority game model Hamiltonian taken with opposite sign. The results are compared with ones in literary sources.

Strong-interaction approximation for transfer-matrix method

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Using transfer-matrix method a correspondence between classical two-dimensional spin systems (two-dimensional Ising model and six-vertex model) and one-dimensional quantum spin systems is considered. We find the transfer matrix in two limits – in a well-known strong-anisotropy limit and a novel strong-interaction limit. In contrast to the usual strong-anisotropy approximation, within the strong-interaction approximation we take into account the non-commutativity of transfer-matrix components. The latter approximation is valid for low temperatures or strong interaction in one spatial dimension. We observe that the Hamiltonian of the corresponding quantum chains contains multispin interactions.

Longitudinal and transverse dielectric, piezoelectric, elastic, dynamic, and thermal properties of the Rochelle salt $NaKC_4H_4O_6 \cdot 4H_2O$

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A four-sublattice order-disorder model with taking into account piezoelectric coupling and external electric fields is developed for description of phase transitions, longitudinal and transverse dielectric, piezoelectric, elastic and thermal properties of the Rochelle salt crystal. Our model is a generalization of four-sublattice model proposed in [1] and Mitsui model with taking into account the piezoelectric coupling [2]. Within a mean field approximation specific heat, dielectric constants $\varepsilon_{11}^{\varepsilon}$, $\varepsilon_{22}^{\varepsilon}$, $\varepsilon_{33}^{\varepsilon}$ for a clamped crystal and $\varepsilon_{11}^{\sigma}$, $\varepsilon_{22}^{\sigma}$, $\varepsilon_{33}^{\sigma}$ for a free crystal, elastic constants c_{44}^{E}, c_{55}^{E}, c_{66}^{E} at constant field and c_{44}^{P}, c_{55}^{P}, c_{66}^{P} at constant polarization, piezoelectric moduli d_{14}, d_{25}, d_{36}, e_{14}, e_{25}, e_{36}, h_{14}, h_{25}, h_{36}, g_{14}, g_{25}, g_{36} are calculated. The calculation of longitudinal and transverse dynamic permittivities is performed within Glauber method with taking into account Newtonian equatin of motion for dynamics of shear strains. The set of the theory parameters providing the best fit to the available experimental data calculated characteristics is found.

[1] I.V. Stasyuk, O.V. Velychko, Ferroelectrics, 2005, **316**, 51.
[2] R.R. Levitskii, I.R. Zachek, T.M. Verkholyak, A.P. Moina, Phys. Rev. B, 2003, **67**, 174112.
[3] R.R. Levitsky, I.R. Zachek, A.S. Vdovych, Preprint of the Institute for Condensed Matter Physics, ICMP-09-02U, Lviv, 2009 (in Ukrainian).

Two-particle electron correlation function of semi-infinite jellium

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Successive theory of description the electronic subsystem of metal requires the correct calculation of correlation functions of electrons, in particular, two-particle [1,2]. In the case of space bounded system the calculation of such functions becomes considerably more complicated. To illustrate this fact it should be mentioned that while there is a simple algebraic equation for a two-particle correlator in boundary homogeneous system [1] (in random phases approximation), in the case of inhomogeneous system there is an integral equation [3] which can be solved only in the some approximation.

A calculation and research of two-particle correlator of interactive electronic subsystem of the semi-infinity metal in random phases approximation is realized in present work. The surface potential is modeled by different model potentials, allowing to find analytical solution to Schrödinger equation. For the first time the electronic states with energy which is higher than the height of a potential barrier in calculation of two-particle correlator are taken into account. The influence of these states on the behaviour of correlation function is also investigated.

[1] Vavrukh M., Paslavskii V., Phys. Status Solidi B. 1998, **208**, 91.
[2] Kostrobij P.P., Markovych B.M., Condens. Matter Phys., 2008, **11**, 641.
[3] Kostrobij P.P., Markovych B.M. AIP Conf. Proc., 2009, **1198**, 78.

Investigation of hierarchical condensation conditions near phase equilibrium

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Novel mechanism of new phase formation is studied both experimentally and theoretically on the example of quasi-equilibrium stationary condensation in ion-plasma sputterer. Copper condensates are obtained to demonstrate that in the course of deposition specific network structure is formed as a result of self-assembly. The fractal pattern related is inherent in the phenomena of diffusion limited aggregation. Condensate nuclei are shown to form statistical ensemble of hierarchically subordinated objects distributed in ultrametric space. The Langevin equation and the Fokker-Planck equation related are found to describe stationary distributions of thermodynamic effect at condensation and corresponding probability current. Time dependence of formation probability of branching structures is found to clarify the experimental situation.

The 36-th Conference
of the Middle European Cooperation in Statistical Physics

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5–7 April 2011, Lviv, Ukraine

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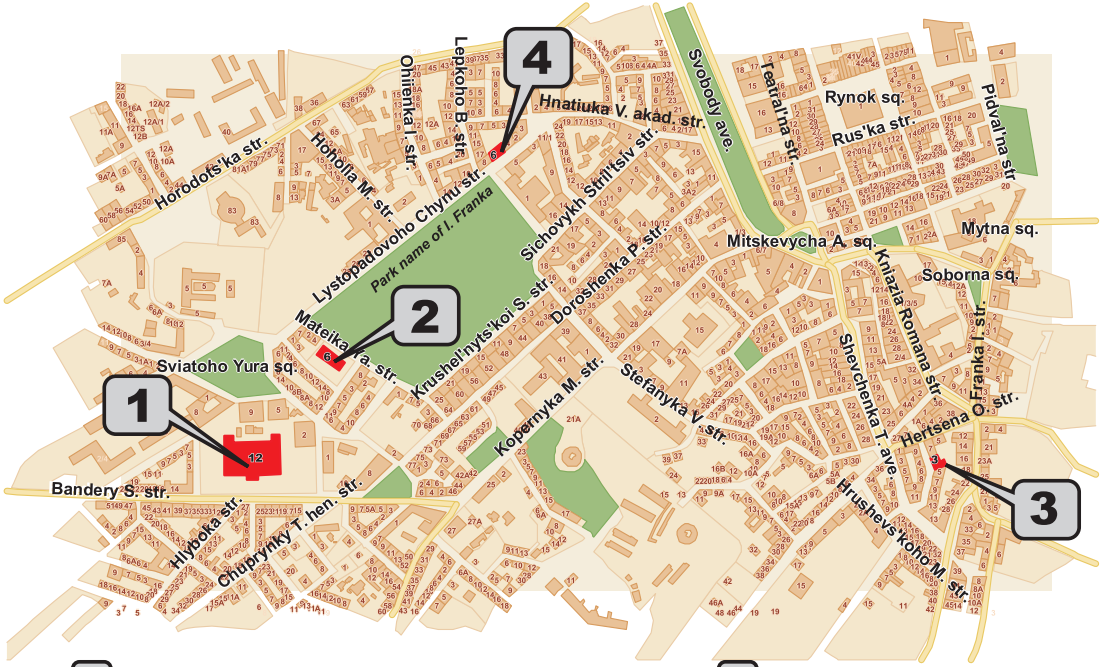
Lviv Map



1 Lviv Polytechnic National University

2 Hotel “Dnister”

3 Ivan Franko Lviv National University Hotel

4 House of Scientists

36-та конференція
центрально-європейської співпраці в галузі статистичної фізики

MECO 36

Львів, 5–7 квітня 2011 р.

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Timetable of the 36-th Conference of the Middle European Cooperation in Statistical Physics

Time	Monday April 4	Tuesday April 5	Wednesday April 6	Thursday April 7
09.10-09.20		Welcome		
09.20-10.00		Y. Imry	J.F. Mendes	A. Ciach
10.00-10.20		L. Cugliandolo	R. Mahnke	D. Mouhanna
10.20-10.40		O. Bakai	R. Kenna	J. Strečka
		Coffee		
11.10-11.50		G. Kahl	C. Bechinger	11.10-11.30 J. Sznajd 11.30-11.50 O. Velychko
11.50-12.10		A. Scala	A. Gambassi	D. Cabra
12.10-12.30		I. Nezbeda		T. Domanski
12.30-12.50			O. Vasilyev	
			Lunch	
14.00-15.30	Registration	Poster	Excursion	Poster
15.30-16.10		H. Zapolsky		A. Chechkin
16.10-16.30		W. Janke		G. Oshanin
16.30-16.50		A. Chalyi		A. Stanislavsky
		Coffee		Coffee
17.20-17.40		P. Viot		A. Savin
17.40-18.00		A. Donoso		L. Banchi
18.00-18.20		G. Gonnella		T.J.G. Apollaro
19.00	Welcome Party	Dinner	Conference Dinner	Dinner