25 August, Saturday
About the reasons of the role of Riemann and Goldbach's hypotheses on the behaviour of complex systems

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The authors have already designed a bi univocal application between Riemann zeta functions and dynamic processes under the control of Integro-Differentiation Operator of Non Integer Complex Order. They show that the Riemann zeta function can then be related to hyperbolic geodesics whose angles at the boundary are determined by the real part of the power laws that define the Riemann series. They suggest that Riemann's conjecture can be reduced to a geometrical phase transition with a reduction of the parameter of order resulting from the combination of a couple of symmetries associated with a quasi self similarity of geodetics. The well known relationship with the set of prime number must be considered as the result of the local existence of stationnary 'state' of the dynamics.

The lecture will focused the topic on the 'non stationary' behaviour of Riemann zeta function. It will be shown that the main characteristic of the dynamics of complex systems, may be associated to a hybridizing between a couple of states and/or processes able to give a geometrical status to the concept of the time and equally to the concept of energy, in spite of the disappearance of the concept of local standard action. It will be shown that the set of prime numbers which focus and polarizes the transitions of ‘states’ is the simplest form of the complexity. This analysis will suggest the existence of a mathematical relationship between Riemann and Goldbach hypothesis.
We assume that there are two key conditions for the implementation of glass transition. First of all, we believe, that the glass transition has common nature with the second order phase transition, which is spontaneous breaking continuous symmetry and starting an ordering process in the system structure. On the other hand, in contrast to the phase transition this ordering process stops because of frustration, which arises in this process. The presence of frustration is the second key condition for glass transition. The frustration gives rise to production of vortexes (spin vortexes in the spin systems, or disclinations in the undercooled liquids [1, 2]) in the structure, which prevents the growth of the ordered regions. The nonequilibrium dynamics of the slowing vortex system, which takes into account the interaction between these vortexes, can be described in terms of the gauge field theory. Therefore the old, and almost forgotten idea of the gauge field description of glass transition underlies in this work [1, 3, 4].

An important point of this theory is the presence of the vortexes in the structure. They can exist without frustration, but then their concentration tends to zero at the phase transition point, in which the relaxation time diverges. We take into account, that additional, induced by the frustration, vortices are present in the structure besides the thermoactivated vortexes. Therefore, close to the glass transition there is a finite nonzero density of vortexes. We believe that above the glass transition temperature the vortices system is in equilibrium. This fact makes it possible to average over the gauge field sources, that results in the temperature displacement of the critical point in the gauge field subsystem. Then we use the renormalization group methods and critical dynamics methods for the description of the static and dynamic properties of the system at the new critical point [5]. In terms of this approach the glass transition corresponds to the critical point in the gauge field subsystem. We examine both the static case and the dynamic case, and show that the theory's linear and non-linear susceptibilities agree with the experimental data. The dynamic features of this transition, such as the Vogel-Fulcher-Tamman relaxation time dependence on temperature, the characteristic temperature dependencies of the heat capacity, and the plateau in the time dependence of the order parameter correlation function, can be revealed by means of the functional methods of non-equilibrium dynamics. In conclusion we consider the relationship of the suggested theory with the mode-coupling theory approach and the frustrated-limited domain theory, and discuss its physical interpretation.

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MOLECULAR DYNAMICS SIMULATION OF THE STEADY-SHEAR FLOW IN MODEL GLASSY MATERIALS

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We have performed the non-equilibrium molecular dynamics simulation of the model glassy Dzugutov system under steady homogeneous shear flow [1, 2]. Our results discover a favorable influence of the external shear of on the structural ordering in the system. Furthermore, the increases of the temperature and of the shear rate promotes the growth of the nucleation rate in the glassy system, where a crystalline clusters growth through the attachment to the nucleus of the monomers. Finally, at the large time scales the glassy phase passes almost completely into the ordering state that is verified by the values of the orientation order parameter $Q_0 \approx 0.45 \pm 0.03$ [3].

Dynamic Processes in Amorphous Metallic Alloys

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We study the structural properties and collective microscopic dynamics in Ni$_{33}$Zr$_{67}$ amorphous metallic alloy by computer atomic/molecular dynamics simulations on the basis of the model pair-wise potential. The calculated equilibrium characteristics are compared with the experimental data on inelastic X-ray scattering. Based on the recurrent relation approach [1], we present the theory of structural relaxation of the microscopic density fluctuations of particles for amorphous metallic alloys. The results of theoretical calculations for the intensity of scattering $I(k,\omega)$ in the amorphous metallic alloy Ni$_{33}$Zr$_{67}$ are in a good agreement with the results of computer simulation as well as with the experimental data on inelastic X-ray scattering [2].

References
An extended mean-first-passage-time approach: 
New tool to treat experimental and simulation results in nucleation-growth kinetics

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We show that the mean-first-passage-time approach \cite{1} could be extended to perform the analysis of the data for nucleation-growth kinetics. The main idea of the approach is to perform the statistical treatment of the independent runs and to focus on the selected set of the reaction coordinates (or order parameters) \cite{2}. The remarkable feature is that this approach allows one to extract practically all the parameters characterizing the initial stages of a phase transition. Moreover, it can be applied to the experimental data as well to the molecular dynamics simulation results \cite{3}.

References

Description of the anomalous dielectric relaxation in disordered systems in the frame of the Mori-Zwanzig formalism

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One of the most striking features of the dielectric relaxation phenomenon in different disordered materials such as glass-forming liquids and amorphous polymers is the failure of the Debye [1] theory. This simple theory of dielectric relaxation cannot describe properly the low-frequency spectrum, where the real relaxation behavior can deviate essentially from the conventional exponential Debye's pattern and actually it is characterized by a broad distribution of relaxation times. Such behavior is reflected in the title anomalous dielectric relaxation and in the first time was suggested empirically in the pioneer paper [2] of the Cole's brothers in 1941 year for description of dielectric relaxation in polar liquids. In the most cases when the non-Debye dielectric spectra are considered the measured data have been described by the so called Havriliak–Negami (HN) relationship suggested as an empirical expression for the complex dielectric permittivity (CDP)

\[ \epsilon^*(\omega) = \frac{\epsilon_\infty - \epsilon_0}{(1 + i\omega \tau)^\beta}, \quad 0 < \alpha, \beta \leq 1. \]  

(1)

Here \( \alpha \) and \( \beta \) are empirical exponents. The partial case \( \alpha=1, \beta=1 \) reproduces the Debye relaxation law, \( \beta=1, \alpha\neq1 \) corresponds to the so-called Cole–Cole (CC) equation, while the case \( \alpha=1, \beta\neq1 \) corresponds to the Cole–Davidson (CD) formula. There is an actual problem of construction the reliable theory that enables to describe the CDP in terms of (1) and find the physical meaning of the empirical power-law exponents \( \alpha \) and \( \beta \) figuring in (1).

In the given paper the authors suggest an original approach for derivation of empirical expression (1) and its partial cases based on the kinetic equations containing the non-integer integrals and derivatives for relaxation function. As the basic structure for derivation of expression (1) it is suggested to use the general kinetic equations suggested by Mori and Zwanzig based on the first principles of the non-equilibrium statistical mechanics. At derivation of the desired kinetic equations we use the self-similar model of dielectric relaxation described in detail in [3]. This model is based on the hierarchy structure of different levels of organization of relaxation process in disordered materials. The model initially constructed for the derivation of the Cole-Cole expression is redefined by introduction of new relaxation mechanisms and uses the memory function of the second order. These modifications allow to derive the desired kinetic equations for the remaining empirical functions CD and HN, correspondingly. The suggested approach is rather general.

It allows to describe not only the anomalous dielectric relaxation having one loss peak (\( \alpha \) - relaxation) but enables also to derive the CDP expressions describing multi-peaks spectra (\( \beta \) - relaxation).

References
We investigate the critical properties of asymmetrical trilayers $F_1F_2S$ and $F_1SF_2$ structures in an external parallel magnetic field. The different mutual orientations of the F layers magnetizations are examined. At this condition the triplet component of the superconducting condensate is arisen [1,2]. Assuming that all F and S layers are dirty, we solve the boundary value problem for the Usadel function [3]. Then we use Gor'kov's self-consistency equation and calculate the critical temperature for both trilayers as function of the F layers thicknesses $d_{f_1,2}$ in external magnetic field $H$ [3].

In particular, we predict the surprising appearance of re-entrant superconductivity with increasing magnetic field.

In the figures (a, b) the dependence of the reduced critical temperature $t_{c,1}^{P(A)} = T_c^{P(A)}/T_c$ on the reduced thickness F$_1$ layer $d_{f_1}/a_{f_1}$ for $\phi = 0^\circ$ (a) and $\phi = 180^\circ$ (b) are shown, $\phi$ is the angle between the directions of magnetizations for the $F_1F_2S$ system in the external magnetic field $h = H/H_c$ ($T_c$ is critical temperature of S metal, $H_c$ is critical parallel field of the thin film, $a_f = v_f/2I$ is spin stiffness length, $v_f$ is Fermi velocity and $I$ is exchange field in the F metal). In figure (c) we plot the angular dependence of the critical temperature. We see that the temperature dependence $t(\phi)$ is not monotonic and it has a minimum at $\phi = 90^\circ$.

The work was partially supported by the Ministry of Education and Science of Russian Federation.

Four-layered ferromagnet/superconductor system in external magnetic field

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The four-layered FMSFMS nanostructure consisting of rather dirty superconducting (S) and ferromagnetic (FM) metals at external magnetic field is studied in framework of the proximity effect theory taking into detailed account of the boundary conditions [1,2]. Note, that earlier [1] the conceptual scheme of new nanoelectronics control device has been proposed. It has up to seven different states and combines in one sample the advantages of two different recording channels. The simple three-layered spin-valves [3-5] were considered as two-state spin switches. The switching of all these devices is performed by small external magnetic field, see for example modern experimental results with complete spin-valve effect [6]. Therefore the magnetic field should be taken into account in consecutive theory. Actually for three-layered FM/S system it was shown in recent theoretical works [7].

In this work we study asymmetrical four-layered structure on the Usadel equation base, the influence of external magnetic field is especially examined. The critical temperature versus applied magnetic field’s magnitude, film’s thicknesses and a transparency of the contacts is calculated. We showed that the phase diagrams of the system under consideration are strongly changed in the presence of external magnetic field. In particular, condition of observability of decoupled superconductivity could be considerably affected. The possible applications to superconducting spintronics are discussed.

References

Spin kinetics in heavy fermion systems

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We present a theoretical investigation of heavy-fermion compounds YbRh$_2$Si$_2$ and YbIr$_2$Si$_2$. The main ingredients for understanding the electron spin resonance (ESR) existence in these systems include the renormalization of the Kondo interaction and the local properties of Yb ions in a crystal electric field. The Kondo effect leads to a common energy scale regulating temperature dependence of different physical quantities. The developed model successfully explains the ESR data in terms of their temperature, angular and magnetic field dependencies [1-4].

Ferromagnetism in defect oxides doped by transition-metals

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Nowadays there exist several models of ferromagnetism in diluted magnetic oxides semiconductors (DMS). Most of researchers associate ferromagnetism with the localized magnetic moments on 3d-impurities which order by indirect exchange interactions. However, there are studies in which ferromagnetism is ascribed to electrons of the defect band of the oxide crystal. Which mechanism of magnetic ordering is realized in a particular system remains an open question. Therefore, the aim of this study is to clarify mechanisms of the long-range magnetic order in defective oxide semiconductors for the case when the impurity is distributed in a sample in the form of a solid solution by substituting cations of the matrix.

We propose a mechanism of long-range magnetic order based on the assumption that the band structure of an oxide semiconductor material has a narrow vacancy band with a sufficiently high density of states at the Fermi level $g(E_F)$, and electron in the band are coupled by the exchange interaction $I$. The band electrons are close to the fulfillment of the Stoner criterion, $Ig(E_F); 1$. We also assume the existence of hybridization between localized impurity electronic states and the electronic states of the vacancy band. This hybridization enhances the exchange interaction in a narrow band, triggering its transition to the ferromagnetic state.

To find the modified criterion of ferromagnetism, we calculated the transverse dynamic susceptibility of electrons in the vacancy band by double-time thermodynamic Green functions:

$$\chi_\perp = \frac{g(E_F)\left(1+c \frac{V_F^2}{(E_F - E_d + I/2 - Un/2)^2}\right)}{1 - Ig(E_F)\left(1+c \frac{V_F^2}{(E_F - E_d + I/2 - Un/2)^2}\right)}.$$  \hspace{1cm} (1)

Here $c$ – the concentration of impurity, $E_d$ – 3d-impurity energy level, $U$ – the Coulomb repulsion energy between electrons on the impurity site, $n$ – the average number of electrons on the impurity site, $V_F$ – matrix elements of hybridization.

Expression for the susceptibility (1) shows that the presence of paramagnetic impurities contributes to the paramagnetic-ferromagnetic transition. In contrast to the Stoner ferromagnetism, ferromagnetism in DMS is heterogeneous and appears only on defect area of a sample. The proposed mechanism of long-range magnetic order has a "trigger" behavior. This means that the ferromagnetism is due to electron vacancy band, and the impurity only contributes to its occurrence. The parameters of the ferromagnet (for example, the magnetic ordering temperature, magnetic moment, coercive force) obtained as a result of such mechanism are determined primarily by the parameters of the narrow vacancy band, rather than the type and concentration (if exceeded the threshold concentration, which may be different for ions of different types) ion implanted into the semiconductor. This behavior is observed in our experiments, in which, after overcoming a threshold concentration, the magnetic ordering temperature, although with a certain spread, does not depend on the concentration routinely embedded ions.
The solitary re-entrant superconductivity in the clean four-layered superconductor/ferromagnet system

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This work develops ideas of preceding works [1,2]: we take into account coupling constant in ferromagnetic metals $\lambda_f$ and pair amplitude change along the F/S interface for four-layered system F'/S/F/S' in the clean limit. We investigate the superconducting critical temperature $T_c$ for four different physical states ($\alpha\beta\gamma$) which differ by phase shift of superconducting order parameters ($\alpha = 0, \pi$) between S and S' layers and angle ($\gamma = 0, \pi$) between magnetizations in ferromagnets F and F'. The superconducting order parameter shift $\beta$ between F and F' layers is always equal 0, because we consider only positive $\lambda_f$. We can continuously control by superconducting properties of system changing the ratio of thicknesses $d_f/d_s$. We predict solitary re-entrant superconductivity that is shown in Fig. 1 (curves a-e) for the simplest 00$\pi$ state. The $T_{c_0}$ is critical temperature of bulk S material. For asymmetrical system F'/S/F/S' we foretell also essential competition between the BCS states (solid lines) and FFLO ones (dashed lines). The $g$ curve relates to symmetrical four layered system when thicknesses $d_f = d_f'$ change synchronically and $d_s = d_s'$. In this case the exchange fields of neighboring F layers compensate each other, and critical temperature reaches the maximum value.

![Phase diagram](image)

Fig. 1 Phase diagram for $\lambda_f > \lambda_f > 0$. The upper panel shows the corresponding dependence of the quasimomentum of pairs in the units of inverse spin-stiffness length $a_f$.  


Static magnetic susceptibility of Kondo lattice compounds YbRh$_2$Si$_2$ and YbIr$_2$Si$_2$

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We have studied the static magnetic susceptibility of the Kondo lattice compounds YbRh$_2$Si$_2$ and YbIr$_2$Si$_2$ on the basis of the local properties of Yb-ions in a crystal electric field. The Kondo interaction was taken into account by the method of renormalization group analysis. The renormalization of the Kondo couplings results in a Curie-Weiss law with a logarithmic temperature dependence of Curie constants and Weiss temperatures. Our results are well consistent with the experimental data on YbRh$_2$Si$_2$ and YbIr$_2$Si$_2$ [1-3] (some of our results were published in [4-5]).

References

The superconducting phase transitions for the asymmetrical FS superlattices with interelectronic interaction in ferromagnet layers

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The superconducting and magnetic states coexistence in the FS superlattice, where F is ferromagnetic metal and is superconductor, is investigated on base of microscopically derived boundary value problem [1,2] for the Eilenberger function. The asymmetrical four-layered structure FSFS' is considered as elementary cell. The second order phase transitions are explored for case of ideal boundary transparencies and clean Cooper limit. Each layer is characterized by its own thickness and electronic structure. Materials are also differed by constants (note that this constant for ferromagnet is nonzero [1]!). It is shown, that 0- and π-phase superconducting states of clean thin superlattices FS are defined by value and sign of electronic correlations in all four layers of elementary cell. The competition between uniform BCS pairing and non-uniform Fulde-Ferrell-Larkin-Ovchinnikov pairing [3,4] are also taken into account.

We predict that the complex system under consideration may have up to 8 different states which are characterized following values: 1) the phase shift $\alpha$ between superconducting order parameters in the S and S' layers 2) the same shift $\beta$ for the F and F' layers, and 3) the angle $\gamma$ between the magnetizations in the F and F' layers. All quantities can take only two values 0 and $\pi$. The $\alpha\pi\gamma$ states possible for case interelectronic repulsion in both F layers can be observed only in special cases in the presence of external magnetic field. Among other states we mark out the $\alpha0\pi$ states that can fully explain two surprising experimental facts observed for symmetrical short range superlattice Gd/La [5,6]. First of them is the complete absence of superconductivity suppression for superlattice states with $\gamma = \pi$, and the second is constant value of critical temperature $T_c = T_c(\text{La}) \approx 5$ K for various thickness of F layers $d_{Gd} = (2-3)d_{La}$. Note that usual theory of proximity effect [7] in that is neglected by interelectronic interaction in F layers is not able to explain these peculiarities.

References

Collective spin excitations in lightly doped cuprates $Y_{1-y}Yb_yBa_2Cu_3O_{6+x}$

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We have shown that collective spin excitations of the paramagnetic ions $Yb^{3+}$ and antiferromagnetic spin waves of the CuO$_2$ planes can appear in lightly doped cuprates $Y_{1-y}Yb_yBa_2Cu_3O_{6+x}$ at $0.4 > x > 0.2$ and in a wide region of the $Yb^{3+}$ ions concentrations due to the exchange coupling between the $Yb^{3+}$ and $Cu^{2+}$ ions. We have found the dependence of their frequencies on wave vectors and the corresponding relaxation rates. At the wave vector $q = 0$ these collective excitation are observable by the electron paramagnetic resonance method. At the very low doping ($x < 0.2$) and low temperatures the main contributions to the EPR linewidth are expected to be from the Suhl-Nakamura interactions of $Yb^{3+}$ ions via the antiferromagnetic spin waves and the usual magnetic dipole-dipole interactions. In the region of doping $0.2 < x < 0.4$ an important contribution to the EPR linewidth comes from the spin polarons created by the electron holes doped into the CuO$_2$ planes. At high temperatures appears additional broadening of the EPR signal due spin-phonon interactions of the $Yb^{3+}$ ions as was shown for the case of higher doping [1]. At $x > 0.4$ the contributions from the Suhl-Nakamura interactions and the spin polarons disappears due to destruction of the long range antiferromagnetic order.

References

26 August, Sunday
Kinetic Theory of Superstatistics

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Complex systems are frequently governed by a mixture of hierarchical dynamics on different time scales. Superstatistics, which is a “statistics of statistics” with several largely separated time scales, aims to describe their nonequilibrium stationary states. Here, employing a prototype system, i.e., a Brownian particle moving through a fluctuating medium with slowly varying inverse temperature, Fokker-Planck theory is developed to establish a kinetic foundation of superstatistics. In this theory, both the velocity of the particle and the inverse temperature are dynamically treated with the help of a Born-Oppenheimer-like adiabatic scheme introducing dynamical hierarchy. It is shown that the Fokker-Planck equation admits as a general solution a superstatistical one. Three major universality classes often observed in nature, i.e., gamma, inverse gamma, and log-normal superstatistics are discussed as special solutions.
Klimontovich’s S-theorem and Stochastic Thermodynamics

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We first show that the system entropy change for the transitions between non-equilibrium steady states arbitrarily far from equilibrium for any constituting process is given by the relative entropy of the distributions of these steady states. Finally, we show the relation of these results in stochastic thermodynamics [1] to Klimontovich’s S-theorem [2], which has been offered as a measure of relative degree of order in the physical systems.

References

Interest Rate Changes and Stock Market Volatility: Recent Evidence from Europe

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In 2007, the subprime crisis triggered a cascade of bankruptcies. The crisis was initially confined to the US but spread over other countries all around the world. Europe was especially affected. The European banking system was especially bitten generating low liquidity and a sharp increase in interest rates. European countries such as Iceland and Ireland were in the frontline of the financial crisis but rapidly contagion reached other peripheral countries.

One of the consequences in Europe of the subprime crisis was economic slowdown and depression, most visible in 2009 and onwards. Governments activated a policy of large scale public investment trying to attenuate the economic slowdown, and budget deficit increased. As a result, government total debts also increased and severe liquidity problems triggered a new crisis known as the sovereign debt crisis (or a W crisis). Some governments delayed the implementation of structural measures to cope with the post-crisis and stimulating economic growth. But the Euro remained strong relative to the US Dollar, deepening the economic problems in the most vulnerable countries. Public finance problems and financial market mistrust in some cases reached the Euro Zone, in particular Greece, Ireland and Portugal. But other countries are on the sight of financial investors and rating agencies, including Spain, Italy and Belgium. The consequence was a sharp increase of short- and long-term Treasury bond rates and bankruptcy perspectives in some countries. At the same time, the prices of financial assets fell down with no surprise.

It is therefore important to understand how much the interest rate change affected financial asset risk, especially in what concerns the stock market. We thus develop a model that relates interest rate changes with stock market volatility and produce forecasts of this impact over the sovereign debt crisis and prospective persistence over time. The results are consistent with observed facts in southern countries and Ireland but some surprises are also evident for Scandinavian economies. Who follows?
A Semi-Markov Model of Customer Lifetime in the Portuguese Fixed Telecommunications Industry

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For the last decade, Portuguese customers of fixed telecommunications have easily switched the provider, which has been very damaging for the business performance. This study aims to develop a survival analysis model of the residential customer churn in this industry in Portugal, which can support managers on customer portfolio management. Our results show that the majority of variables that influence customer churn are related to the customer spending with the firm. We also found that the probability of a customer to defect is neither constant over time nor across customers. Lastly, it seems that satisfaction does not influence customer churn.
The zeroth law in nonadditive thermodynamics

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The general functional form of those nonadditive composition rules that are compatible with the zeroth law of thermodynamics are derived and some consequences are calculated. One finds that this general form is additive for the formal logarithms of the original quantities and the familiar relations of thermodynamics apply to these. This result offers a possible solution to the long-standing questions about equilibrium between extensive and nonextensive systems or systems with different nonextensivity parameters. Examples from heavy ion physics are shown.
Group, geometry and algebra of nonextensive entropies in complex systems

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The Abel entropy group and its matrix representation with the general law of nonextensive entropy composition and quadratic nonlinearity are defined. Four types of matrices for the corresponding parametrical entropies are given and geometries for their measures are determined. Algebraic representation of an entropy group is presented for this types of the general entropy classification in statistical thermodynamics of complex systems. The corresponding geometries are global Finsler ones. The well-known relations for the nonextensive entropies follow from the properties of the conformally generalized hypercomplex numbers.
Systems and models with anticipation in physics and its applications

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Investigations of recent physics processes and real applications of models require the new more and more improved models which should involved new properties. One of such properties is anticipation (that is taking into accounting some advanced effects).

It is considered the special kind of advanced systems – namely a strong anticipatory systems introduced by D. Dubois. Some definitions, examples and peculiarities of solutions are described. The main feature is presumable multivaluedness of the solutions.

Presumable physical examples of such systems are proposed: self-organization problems; dynamical chaos; synchronization; advanced potentials; structures in micro-, meso- and macro- levels; cellular automata; computing; neural network theory. Also some applications for modeling social, economical, technical and natural systems are described.
Study of energy fluctuation effect on the statistical mechanics of equilibrium systems

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It is known that when an equilibrium system gets smaller and smaller, one of the major quantities that become more and more uncertain is its internal energy. These increasing fluctuations can considerably modify the original statistics. In works \cite{1, 2} the relations between energy variance and heat capacities have been used to study relationship between fluctuations and negative specific heat.

In the present work we report about modeling of energy fluctuation effect on the behavior of small classical thermodynamic systems. The present model focuses on the effect of these energy fluctuations by consideration an overlap between the Boltzmann-Gibbs statistics and the statistics of the fluctuations. Within this “overlap statistics”, we studied the effects of several types of energy fluctuation on the probability distribution, internal energy and heat capacity.

It is shown that the fluctuations can considerably change the temperature behavior of internal energy and heat capacity in the low energy and temperature region. Particularly it has been found that, due to the lower energy limit of the systems, the fluctuations reduce the probability of the low energy states (Fig.1) and increase the total average energy. Such energy increasing is more pronounceable for lower temperatures, making negative heat capacity possible for low temperature region (Fig.2).

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{Fig1.png}
\caption{Probability distribution for 2D free particle in case of q-Gaussian fluctuation distribution for different q at temperature $\theta = 1$ and $\sigma = 1$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{Fig2.png}
\caption{Heat capacity of 2D free particle in case of q-Gaussian fluctuation distribution for different values of q = 3/2, 7/4, 15/8, 19/10, 31/16 from top to bottom ($\sigma = 1$).}
\end{figure}

References

Entropy: A new measure of stock market volatility?

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When uncertainty dominates understanding stock market volatility is vital. There are a number of reasons for that. On one hand, substantial changes in volatility of financial market returns are capable of having significant negative effects on risk averse investors. In addition, such changes can also impact on consumption patterns, corporate capital investment decisions and macroeconomic variables. Arguably, volatility is one of the most important concepts in the whole finance theory. In the traditional approach this phenomenon has been addressed based on the concept of standard-deviation (or variance) from which all the famous ARCH type models – Autoregressive Conditional Heteroskedasticity – depart. In this context, volatility is often used to describe dispersion from an expected value, price or model. The variability of traded prices from their sample mean is only an example. Although as a measure of uncertainty and risk standard-deviation is very popular since it is simple and easy to calculate it has long been recognized that it is not fully satisfactory. The main reason lies on the fact that it is severely affected by extreme values. This may suggest that this is not a closed issue.

Bearing on the above we might conclude that this is not a closed issue and that many other questions might arise while addressing this subject. One of outstanding importance, from which more sophisticated analysis can be carried out, is how to evaluate volatility, after all? If the standard-deviation has some drawbacks shall we still rely on it? Shall we look for an alternative way? In searching for this shall we consider the insight of other domains of knowledge? In this paper we specifically address if the concept of entropy, originally developed in Physics by Clausius in the XIX Century, can constitute an effective alternative. Basically, what we try to understand is what are the potentialities of entropy compared to the standard deviation. But why entropy? The answer lies on the fact that there are already some research on the domain of Econophysics that points out that as a measure of disorder, distance from equilibrium or even ignorance [1], [2] entropy might present same advantages. However another question arises: since there are several measures of entropy which one since there are several measures of entropy, which one shall be used? As a starting point we discuss the potentialities of Shannon entropy, Renyi entropy and Tsallis entropy. The main difference between them is that both Renyi and Tsallis are adequate for anomalous systems while Shannon has revealed optimal for equilibrium systems.

References

Log-periodic oscillations in the specific heat of self-similar spin system of the Ising-type

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Log-periodic oscillations constitute a general property of systems with discrete scale invariance \cite{1}. They have been reported in many different systems where there is a discrete scale invariance in the lattice on which the model considered is defined (e.g. geometric fractals), or it can be defined on the coupling constants appearing over the Euclidean lattice, or in the both cases, simultaneously. The most intriguing appearance of the log-periodic phenomenon is observed in the temperature behavior of the specific heat for quasi-periodic structures, e.g. in quasi-crystals, having the fractal energy spectrum \cite{2}.

In this paper the authors consider the physical system of another type. This system admits the log-periodic behavior of the specific heat also. We consider a model of spin-system which is located in a medium having liquid-type structure and this medium can transmit a specific force (pressure) through the structure. Under external tension is applied in the medium the non-equilibrium state is created and because of its specific property (nonergodicity) the distribution of a heterogeneous pressure over the sample considered can be created. It is supposed the hierarchy-type pressure distribution can be created in glass-forming systems. Taking into account that the value of the exchange integral depends on the values of the external pressure applied one can get finally the self-similar ensemble of spin complexes/clusters which are differed from each other by the value of the exchange integral and number of spins captured by this interaction. Mathematically, these values are subordinated to the following self-similar conditions:

\[ N_l = N_0 b^l, \quad J_l = J_0 \xi^l, \quad 0 < b < 1, \xi > 0, \quad 0 < l < \infty \]

where the values \( N_0, J_0, b, \xi \) define the parameters of the model considered. Then we realize the averaging procedure of the specific free energy over all spin complexes and present the expression for the total free energy as

\[ \overline{f}(\overline{\beta}) = \frac{1}{N} \sum_l N_l f_l(\overline{\beta}, J_l). \]

The last expression allows to restore easily the dependence of the specific heat on temperature. In order to demonstrate the general properties of the log-periodic oscillations and possibilities of the approach suggested we chose the spin system of the Ising type with \( s = \frac{1}{2} \) and the interaction of each spin is realized only with two neighbors (the linear Ising model).

Finally it was shown that the temperature behavior of the model considered has log-periodic oscillations which are combined with monotone power-law dependence \( T^d \), where the value \( d = \pm \ln(1/b)/\ln\xi > 0 \) defines a specific "fractal dimension" of the self-similar ensemble of spin complexes.

References

27 August, Monday
To Be Announced

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Critical fluctuations for 1D Bak-Sneppen model

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A dynamical model for hierarchy and modular organization: The trajectories en route to the attractor at the transition to chaos

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We show that the comprehensive features [1] of the dynamics towards the Feigenbaum attractor, present in all low-dimensional maps with a unimodal feature, form a hierarchical construction with modular organization that leads to a clear-cut emergent property. This well-defined nonlinear model system combines a simple and precise definition, an intricate nested hierarchical dynamical structure, and emergence of a power-law dynamical property absent in the exponential-law that governs the dynamics within the modules. This classic nonlinear system is put forward as a working example for complex collective behavior.

Reference
To Be Announced

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I-theorem and self-organization in the van der Pol generator

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Based on the S- and I-theorems of evolution of $q$ entropy and $q$ discrimination information, the process of self-organization developing in the van der Pol generator with variation of the feedback parameter at induced transitions between stationary states in an open nonextensive system is studied.
The BigDFT code as an efficient tool for nanoscience

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Recently, computer modelling and simulations at the atomic level acquires greater importance in many fields of science: physics, material science, biology, and chemistry. The Kohn-Sham formalism in the approximation of the density functional theory is the most widely used first-principle method for treating atomic systems. One of the important components for the solution of Kohn-Sham equations is the set of basis functions. Currently the plane waves basis set is used in most DFT codes for solid-state physics. The ab initio BigDFT code uses the wavelets as a basis set of wave functions. Due to the fact that Daubechies wavelets are localised and orthogonal both in real and Fourier space the attractive possibility of effective treatment of nonperiodic or inhomogeneous systems as well as surfaces appears [1].

It is known that for most codes the number of computational operations raises cubically with the number of electrons. As a result, the consumption of computing resources to operate the system with larger than several tens of atoms is a serious restriction on the possible size of the system. However the implementation of the full electronic structure calculation BigDFT code on a hybrid parallel architecture with Graphic Processing Units shows very good performances, systematic convergence properties and an excellent efficiency on parallel computers. The code is able to run on many cores which may or may not have a GPU associated. With double precision calculations, the considerable speedup between a factor of 20 for some operations and a factor of 6 for the whole DFT code may be achieved [2].

Of special interest is the recently implemented Activation-Relaxation Technique which allows to study the energy surface of the system (saddle points and local minima). Combination of Lanczos algorithm with the direct inversion in interactive subspace scheme (DIIS) makes possible to generate events to go from initial minimum through a saddle point up to a final minimum. The possibility to find the saddle point is due to the DIIS procedure which is assured to converge to the closest critical point (e.g. saddle, shoulders, or minima) [3].

In other words this code shows high systematic convergence properties, very good performances and an excellent efficiency for parallel calculations. And as a result the possibility to sample the energy surface and reaction pathways for complex systems becomes real. So the BigDFT code can be a very efficient driving force to develop and advance the nanoscience.


Ab initio studying of topological insulator Bi$_2$Se$_3$ under the stress

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A topological insulator is an unusual state of quantum matter which, while being an insulator in the bulk, has topologically protected electronic states at the surface [1,2]. These states could be probably used in different applications, such as spintronics and quantum computing. However, in transport measurements, it has proven difficult to disentangle the surface contribution from the bulk conductivity, which is substantial even in the lowest carrier density samples. To distinguish surface and bulk contributions into transport properties an external pressure could be applied [3].

In the present work we have performed ab initio calculations of topological insulators Bi$_2$Se$_3$ under the strain. Calculations have been performed by means of DFT approach with exchange-correlation functional PBEsol [4] and with taking into account the spin-orbit interaction, which is realized in the VASP code[5].

Fig.1 Band structure near Gamma point for surface at different pressures

It was found that topologically protected surface states do not change under the hydrostatic pressure (see Fig.1). Moreover, pressure tends to increase electronic density of states in the bulk of Bi$_2$Se$_3$. In addition, the hole pocket which is bulk localized was found at high pressure (see Fig.2). Probably, it could be the sign of the metal-insulator phase transition of Bi$_2$Se$_3$.

Thus, the results of ab initio calculations could complement the experimental investigations of high pressure transport properties in topological insulators samples and the experimentally detected growth of carrier density could be related to the bulk transport properties. Nevertheless, additional calculations should be performed in order to determine the reason of hole pockets and to give the explanation of experimentally detected electron mobility dependence [3].

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Ab initio investigation of properties of fluoride scheelite LiGdF$_4$ under pressure

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In this work, the response of LiGdF$_4$ compound on the pressure is considered in the light of the recently reported high-pressure X-ray diffraction data [1]. LiGdF$_4$ is a positive uniaxial crystal with tetragonal scheelite symmetry commonly used as a laser host material. The investigations structural and mechanical properties of LiGdF$_4$ compound were carried out using DFT as implemented in Vienna Ab-Initio Simulation Package (VASP 5.2) [2], part of the MedeA® modeling interface. The exchange–correlation functional was approximated by the gradient corrected form proposed by Perdew-Burke-Ernzerhof (PBE) [3]. The electronic degrees of freedom were described using the projector augmented wave method (PAW) and basis of plane waves as implemented in VASP 5.2 [4]. MedeA® MT module was used for the investigation of mechanical properties. Non magnetic, spin polarized, spin orbit coupling methods were considered as well as the f-electrons of Gd kept frozen in the core or included in the valence states.

A good agreement of structural (Fig.1) and mechanical parameters with experimental values [1] was obtained. The compression data (obtained by non magnetic method) which are fitted by a Birch–Murnaghan equation of state, gives the zero-pressure bulk modulus 78.9 GPa and the unit-cell volume of scheelite at ambient pressure 302.4 Å$^3$.

Fig.1 Evolution of $a$, $c$ parameter versus the pressure (non magnetic core-solid square, spin polarized core-solid triangle, spin polarized valence-blank triangle, spin orbit core-solid circle, spin orbit valence-blank circle, experimental data [1] -solid rhomb.

MT module calculations show the instability of the structure at 10 GPa. This result is in accordance with the experiment which shows the decomposition of the structure near 11 GPa.

References


Ab initio investigation of properties of fluoride scheelite LiLuF$_4$ under pressure

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The interest to the LiLuF$_4$ compound was invoked by the fact that this material possesses the own electrical dipole moment in some temperature range. LiLuF$_4$ compound has been experimentally investigated up to 19.5 GPa [1]. At 10.7 GPa this material undergoes a tricritical phase transition to the fergusonite structure (C12/c1, Z = 4) and the nature of this ferroelastic phase transition is still under the question.

We performed ab-initio calculations by means of DFT [2] with using VASP 5.2 [3] (Vienna Ab-Initio Simulation Package) program, the part of the MedeA$^\text{®}$ interface. The exchange-correlation functional was approximated by the gradient corrected form proposed by Perdew-Burke-Ernzerhof (PBE). The electronic degrees of freedom were described using the projector augmented wave method (PAW) and basis of plane waves as implemented in VASP 5.2. The application of DFT method to d-electrons gives the divergence with experimental results. Due to this simplified LDA (Local Density Approximation) + U scheme was used, where U is Habbard parameter. The several Habbard parameters were considered, but the most suitable parameter is equal to 1 eV.

We have analyzed the structure parameters of LiLuF$_4$ for two possible crystal symmetries I4$_1$/a and C12/c1 versus the pressure (Fig.1). The structure with C12/c1 symmetry transforms to the structure with I4$_1$/a symmetry at pressure near 10.5 GPa.

![Normalized lattice parameters](image)

Fig.1. Pressure dependences of lattice parameters (C12/C1 symmetry) normalized to the respective value at ambient pressure (experimental values [1]: empty square- c$_0$/c$_0$, empty rhomb- a$_0$/a$_0$, empty triangle- a$_m$/a$_0$, empty inverse triangle- b$_m$/c$_0$, empty circle- c$_m$/a$_0$; ab-initio calculations: solid rhomb- a$_m$/a$_0$, solid square- b$_m$/b$_0$, solid circle- c$_m$/c$_0$); the angle of C12/c1 structure versus the pressure (m-monoclinic symmetry, t-tetragonal symmetry).

The combined volume compression data for the scheelite and fergusonite symmetry of LiLuF$_4$ up to 20 GPa was fitted by a common Birch–Murnaghan equation of state and give unit cell volumes (283.3 Å$^3$, 282.3 Å$^3$, respectively) at ambient pressure which are in a good agreement with experimental results [1].

References
Prediction of thermodynamic properties of natural gases by Monte Carlo simulation

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Despite the large amount of experimental data in the literature, the oil and gas industry faces several problems related to correct description of the heavy hydrocarbons. Equations of state have limited application area and discordances with some experiments. Often experiments are not commercially or technically available.

In comparison with last ones molecular simulation does not have such limitations. It is efficient tool to solve many problems related to predict thermophysical properties in a single theoretical framework, which is statistical thermodynamics, in a wide range of temperature and pressure. Molecular simulation is an emerging technique which consists in performing a detailed simulation of microscopic systems involving typically a few hundreds of molecules. The simplest calculations can be performed by hand, but inevitably computers are required to perform molecular modeling of any reasonably sized system. There is several ways to modeling depending on system size. In our work we deal with big systems (rather than thousand atoms) and we use Monte Carlo simulation. Moreover we have an opportunity to compare calculation results with experimental measurements.

In the present work an overview of Monte-Carlo simulation applications for oil and gas production is presented as well as investigation of model of natural gas of the Bavlinskoe reservoir. For this natural gas and for pure gases of methane and ethane we obtained thermal expansivity, isothermal compressibility, compressibility factor, heat capacities, Joule–Thomson coefficient and densities at pressures up to 110 MPa at reservoir temperature. Also we obtained liquid-vapor phase diagrams, critical temperature and pressure and liquid – vapor pressure curves. Predictions for methane are in good agreement with respect to the experimental data.