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Transportation Dynamics on Mobile Node Network

Bing-Hong Wang ¹)

¹) Department of Modern Physics, University of Science and Technology of China, Hefei 230026, China
email: bhwang@ustc.edu.cn

We introduce a model to explore the basic physics of transportation on mobile node networks. Of particular interest is the dependence of the throughput on speed of agent movement and communication range.
The scaling of the dynamical weighted public transport networks in China

Long Guo\textsuperscript{1)}, Yueying Zhu\textsuperscript{2)}, Zhongjie Luo\textsuperscript{1)}, Wei Li\textsuperscript{2)} and Xu Cai\textsuperscript{2)}

\textsuperscript{1)}School of Mathematics and Physics, China University of Geosciences(Wuhan), 430079, Lumo Road, Wuhan, China.
\textsuperscript{2)}Institute of Particle Physics and Complexity Science Center, Central China Normal University, 430079, Luoyu Road, Wuhan, China.
e-mail:zhuyy@iopp.ccnu.edu.cn.China

In this paper, we focus on the topological structure of the four dynamical weighted public transport networks in China in space L. The weighted values of nodes and edges are dependent on the number of the real bus routes. We find the distributions of the weights of nodes and edges, the correlation between nodes follow the power law functions, which are independent of the details of cities. Furthermore, we analyze the fractal dimensions of these public transport networks using the method introduced by Shanker, and find that the average ‘density’ follows a better power-law function as a function of distance \(r\) with the exponent close to 2, which is independent of the real bus routes and reflects the universal spatial properties of the public transport networks in Space L. Our present works provides some new perspective and tool to realize the human dynamics on spatial networks.

Reference

Universal Scaling in Sports Ranking

Li Wei

1) Institute of Particle Physics Hua-Zhong Normal University Wuhan, 430079, Wuhan, China.
E-mail: liw@phy.ccnu.edu.cn

Ranking is a ubiquitous phenomenon in human society. By clicking the web pages of Forbes, you may find all kinds of rankings, such as world’s most powerful people, world’s richest people, top-paid tennis stars, and so on and so forth. Herewith, we study a specific kind, sports ranking systems in which players’ scores and/or prize money are accrued based on their performances in attending various matches. By investigating 40 data samples which span 12 different sports fields, we find that the distributions of scores and/or prize money follow universal power laws, with exponents nearly identical for most sports fields. In order to understand the origin of this universal scaling we focus on the tennis ranking systems. By checking the data we find that, for any pair of players, the probability that the higher-ranked player tops the lower ranked opponent is proportional to the rank difference between the pair. Such a dependence can be well fitted to a sigmoidal function. By using this feature, we propose a simple toy model which can simulate the competition of players in different matches. The simulations yield results rather consistent with the empirical findings. Extensive simulation studies indicate the model is quite robust with respect to the modifications of some parameters.
Empirical mode decomposition for ECG analysis

A. Gizatullin$^1$, D. Tayurskii$^1$

$^1$Institute of Physics, Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia
e-mail: amirgizat@gmail.com

The electrocardiogram is the main method of diagnostics in cardiology. It is very popular because this method is not invasive, effective and rather cheap. Nowadays scientists try to create the effective automatic computerized analysis of ECG signals. All existing methods are based on apriori basis. The most popular method based on wavelet analysis. If a wavelet well suits one patient, then it does not mean that this wavelet will suit other patient.

Any ECG signal contains peaks, segments and intervals. The cardiologist without effort can define these sites. However for the automatic computer analysis their detection is the main objective.

In the present work we consider the method of detection of R, Q wave and the PR, QRS, RR intervals. This method based on the empirical mode decomposition (EMD) of the signal [1]. The main feature of this method is an adaptability - it doesn’t depend from apriori basis. Any non-stationary and nonlinear signal is exposed to decomposition that makes it the universal tool for the analysis of real data. The EMD is adaptive iterative computing procedure of decomposition of signal on intrinsic mode functions (IMF). Thus, the EMD decomposes a signal in finite sum of IMFs which form an orthogonal system. The partial sums of IMFs form components of this signal.

The empirical mode decomposition is based on the three assumptions: the signal has at least two extrema - one maximum and one minimum; the characteristic time scale is defined by the time lapse between the extrema; if the data were totally devoid of extrema but contained only inflection points, then it can be differentiated once or more times to reveal the extrema. Final results can be obtained by integration(s) of the components.

We get the components of signal after applying the empirical mode decomposition for ECG signal. For the analysis of the ECG signal we used the first two IMFs. The sum of the first components of the empirical mode decomposition defines the position of the peak R and PR, QRS, RR intervals on the time axis. So, adding the first two IMFs we received a basic curve. The local maxima and minima, and the intersection with the time axis the basic curve, which will allow us to determine the position of the peaks and the boundaries of the intervals.

The above method was tested on synthetic and real ECG signals from the database PhysioBank.

Reserves Represented by Random Walks

J. A. Filipe 1), M. A. M. Ferreira 1), M. Andrade 1)

1) Instituto Universitário de Lisboa (ISCTE-IUL), BRU-IUL, Lisboa, Portugal
email: jose.filipe@iscte.pt

The reserves problem is studied through models based on Random Walks. Random walks are a classical particular case in the analysis of stochastic processes. They do not appear only to study reserves evolution models. They are also used to build more complex systems and as analysis instruments, in a theoretical feature, of other kind of systems. In this work by studying the reserves, the main objective is to see and guarantee that pensions funds get sustainable. Being the use of these models considering this goal a classical approach in the study of pensions funds, this work concluded about the problematic of reserves. A concrete example is presented.
Representation of Reserves Through a Brownian Motion Model

M. Andrade\(^1\), M. A. M. Ferreira\(^1\), J. A. Filipe\(^1\)

\(^1\) Instituto Universitário de Lisboa (ISCTE-IUL), BRU-IUL, Av.ª das Forças Armadas, 1649-026, Lisboa, Portugal.
e-mail: marina.andrade@iscte.pt

The Brownian Motion is commonly used as an approximation for some Random Walks and also for the Classic Risk Process. As the Random Walks and the Classic Risk Process are used frequently as stochastic models to represent reserves, it is natural to consider the Brownian Motion with the same purpose.

In this study a model, based on the Brownian Motion, is presented to represent reserves. The Brownian Motion is used in this study to estimate the ruin probability of a fund. This kind of models is considered often in the study of pensions funds.

References

Studying Pensions Funds through an Infinite Servers Nodes Network: A Theoretical Problem

M. A. M. Ferreira¹, M. Andrade¹, J. A. Filipe¹

¹ Instituto Universitário de Lisboa (ISCTE-IUL), BRU-IUL, Av.ª das Forças Armadas, 1649-026, Lisboa, Portugal.
e-mail: manuel.ferreira@iscte.pt

This study intends to present a representation of a pensions fund through a stochastic network with two infinite servers nodes. With this representation it is allowed to deduce an equilibrium condition of the system with basis on the identity of the random rates expected values, for which the contributions arrive to the fund and the pensions are paid by the fund. In our study a stochastic network is constructed where traffic is represented. This network allows to study the equilibrium in the system and it is admissible to get a balance to a pensions fund.

A specific case is studied. When the arrivals from outside at nodes A and B are according to a Poisson process, with rates $\lambda_A$ and $\lambda_B$, respectively, the system may be seen as a two nodes network where the first node is a $M/G/\infty$ queue and second a $M/G/\infty$ queue. For this case in the long term the conditions of equilibrium are as follows: $m_A \lambda_A \alpha_A = m_B (p \lambda_A + \lambda_B) \alpha_B$. In this formula it is established a relationship among the two nodes. Several examples are given in the study.

References

The performance of a two-state quantum heat engine improved by the superposition effect

Congjie Ou\textsuperscript{1)}, Jincan Chen\textsuperscript{2)}

\textsuperscript{1)}College of Information Science and Engineering, Huaqiao University, Xiamen 361021, People’s Republic of China.
\textsuperscript{2)}Department of Physics, Xiamen University, Xiamen 361005, People’s Republic of China.
e-mail: jcou@hqu.edu.cn

The performance of a two-state quantum heat engine is analyzed in present paper. It is shown that the efficiency of the heat engine can be enhanced by superposing the eigenstates at the beginning of the cycle. The efficiency of operating the cycle without superposition effect is in fact the lower bound. By employing the finite-time movement of the potential wall, the power out-put of the quantum engine can be analyzed. The results indicate that the superposition effect will enlarge the optimal operating region of the engine. Furthermore, a generic power law potential is adopted to describe this kind of two-level quantum engine in a unified way. The result shows clearly that the performance of the engine depends on the external potential, the geometric configuration of the engine, and the superposition effect.
Ab-initio investigation of the electronic disproportionation in sodium cobaltates

Y.V. Lysogorskiy\textsuperscript{1,2)}, O.V. Nedopekin\textsuperscript{2)}, S.A. Krivenko\textsuperscript{2)}, D.A. Tayurskii\textsuperscript{2)}, and B. Minisini\textsuperscript{1)}

\textsuperscript{1)} Institut Superieur des Materiaux et Mecaniques Avances du Mans, 72000, 44 Av. Bartholdi, Le Mans, France
\textsuperscript{2)} Institute of Physics, Kazan Federal University, 420008, Kremlyovskaya St. 18, Kazan, Russia.
e-mail: s.a.krivenko@mail.ru

With first principle calculations, we have investigated effects of Na\textsuperscript{+} ions ordering on electronic states of the CoO\textsubscript{2} slabs in the lamellar oxide Na\textsubscript{x}CoO\textsubscript{2} for x=2/3 at T = 0. Experimentally, the Na ions become arranged in the positions Na1 and Na2 between the Co plains when the temperature decreases below few hundred Kelvins [1, 2]. This transition is followed by a specific low temperature metallic phase with a substantial site disproportionation, irrelevant for Fermi liquid, when the 3d electrons are segregated between the Co1 and Co2 sites of the triangular Co lattice [1]. The extended spin-active holes Co\textsuperscript{3.44+}, repelled from the inert Co\textsuperscript{3+} sites Co1 adjacent to the Na\textsuperscript{+} cations, are almost confined in the kagomé sublattice Co2. The itinerant magnetic moments ≈1\textmu_B are unusually large, and the ground state of the spins is ordered being the A-AFM phase with the ferromagnetic planar arrangement [2].

A relevant description of the puzzling metal represents a problem. Previous approaches, e.g. [3], rely on the collective effects of the strong Coulomb repulsion in the cobalt 3d-shells of “virtual crystals,” taking a uniform charge background instead of the explicit Na\textsuperscript{+} ions. Then, in the LDA+U approximation [3] the local correlations were established to be optimized by the honeycomb charge ordering when U > 3 eV. However, a large charge gap opens at once at the Fermi level, and the metal becomes an insulator.

To resolve this problem, we have investigated a cooperation of the two mechanisms, both promoting an inhomogeneity of the electronic system: (i) the electron correlations within the 3d shells and (ii) their coupling to the regular superstructure of the Na\textsuperscript{+} ions. Starting with the experimental crystal supercell [1], we have analyzed the electronic states within the GGA+U approximation in a dependence on U. The substantial disproportionation of the magnetic (and valence) 3d states has been revealed between the Co1 and Co2 sublattices when U > 4 eV, see the Figure. The A-AFM spin ordering was established to simultaneously arise. The metallic state was found to be robust up to the realistic value U ≈ 5.5 eV. Our result indicates the crucial role of the Na\textsuperscript{+} superstructure in Na\textsubscript{x}CoO\textsubscript{2}, which controls the frustrated 3d electron on the triangular lattice providing the choice of the peculiar metallic phase from the numerous low-energy states.

The work has been supported by the RFBR under the project No. 10-02-01005-a.

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30 August, Thursday
What we are living for? - Does science (want to) know?

Zbigniew R. Struzik 1)

1) University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8654, Japan
e-mail: z.r.struzik@p.u-tokyo.ac.jp

Asking this question may border either on the irreverent or on existential despair. Yet pondering this subject likely absorbs every single human life, and has possibly infused the realm of humanity since its very beginnings. Oftimes, this question has been (exclusively) apportioned to the realms of religion, the arts and philosophy.

Yet the advance of the exact sciences in the past century could break this conceptual monopoly and open the debate within the verifiable domains of exact sciences previously restricted to non-living matter.

Since the turn of the millennium, the science of living systems has steadily been becoming dominant, with several disciplines raising questions considered to be intractable - as were the fundamental building blocks of matter, two hundred years ago, or the evolution of the universe, a hundred years ago.

Recent advances in bioinformatics, in particular neuroscience and information science as applied to the genetic make-up of life, the science of modelling and explaining adaptation, evolution and emergence, have advanced our conceptual understanding of life’s mechanisms, possibly revealing an opportunity to interpret life's very meaning.

Physics is essential to these developments, I will argue. In particular applications of physics to exotic domains, such as the physics of human interactions - sociophysics, or the monetary aspect of such interactions - econophysics, have been flourishing in recent decades. The borders between such disciplines involved in the 'physics of life' have become less clear-cut than we were used to in the science of 20th century. With recent advances in the exchange of scientific information, a Renaissance polymath type of science is again possible. Indeed, the 21st century has already been dubbed the century of 'the renaissance of science'.

But, given this, will it be possible in our lifetime to ask the profound, eponymous question -the title of this talk- in the context of science?
Spectral analysis on biology networks

Jiao Gu

1)Max Planck Institut fuer mathematik in den Naturwissenschaften, 04103, Inselstrabe, 22, Leipzig, Deutschland.
e-mail: gujiaoocc@gmail.com

We want to find a proper metric to measure the difference between networks, not from matrices directly, since the real network is so always huge. Based on previous research, we know the spectrum reflects structure information of a graph. That is why we choose spectrum as a starting point to explore a proper metric on the space of networks or an algorithm comparing networks. In fact, we hope to prove the spectrum indeed include enough information of the networks. It would be much easier and more convenience to be used.
Reconstruction of neuronal pathways of the brain using diffusion MRI data

A.R. Nasretdinov$^{1)}$, K.A. Il'yasov$^{1)}$, O.V. Nedopekin$^{1)}$

$^{1)}$Institute of Physics, Kazan Federal University, 420008, Kremlyovskaya St.,18,, Kazan, Russia.

Magnetic resonance tractography is a good non-invasive tool for obtaining information on the connectivity between brain regions [1]. Used methods of pathways reconstruction precisely describe its anatomical structure, but are prone to errors associated with the effect of partial volume averaging and noise. By itself, tractography is quite subjective, as it is the only non-invasive method of reconstruction of the pathways in vivo [2]. Since you can not exactly reproduce the actual trajectory of water diffusion on the basis of diffusion-weighted data along the fibers of the neuronal pathways, each path associate must be received by the parameter that characterizes the probability of a given implementation.

In this work we propose a method of neuronal pathways reconstruction using A-star algorithm, with the possibility to assess its the effectiveness. One of the criteria is the probabilistic search parameter G, defined by a set of diffusion coefficients in a given volume element. The parameter G obtained trajectory correlated to its length has the meaning of entropy and allows to assess reliability of the found path.

The proposed method was tested on simulated data with the characteristic behavior of trajectories of the complex variations, different cases of intersection of the beams passing through the intersection without a common voxels, and obtained characteristics of the corresponding probability.

References

Conductivity in porous structures: Verification of the generalized Jonscher's law on different experimental data set

I.I. Popov, R.R. Nigmatullin, A.A. Khamzin, I.V. Lounev

Kazan (Volga Region) Federal University, 420008, Kremlevskaya 18, Kazan, Russia.
e-mail: ii.popov@bk.ru

In paper [1] the new theoretical expression related to the Jonscher's correction for the complex conductivity that determines the contribution of a group of carriers in frequency region has been derived. It has been shown that the conventional Jonscher's term in conductivity represents itself the partial case of more general expression, which is determined by us as the Jonscher's generalized law for conductivity for a wide class of disordered media

\[ \sigma(\omega) = \sigma_0 + \frac{\chi_2 \tau^{-\nu}}{1 + (i\omega\tau)^{-\nu}}. \]

In the low-frequency range when \( \omega \rightarrow 0 \) the suggested expression is reduced to the conventional Jonscher's expression, i.e. \( \lim_{\omega \rightarrow 0} \sigma(\omega) = \sigma_0 + \chi_2 (i\omega)^{-\nu} \). The basic idea that was used for the derivation of the new law is based on the supposition that the disordered medium considered has self-similar (fractal) property [2, 3]. It is natural that this supposition should lead to the idea that the generalized Jonscher's law might be observed in wide a class of disordered materials.

This supposition urged the authors of this paper to more attentive reading of scientific articles where experimental data for the complex conductivity (or the complex permittivity) are collected. These different data would help us to confirm or reject the hypothesis of "universality" that can be associated with the generalized Jonscher's law. In the result of analysis of various experimental data the convincing evidences have been found that the generalized Jonscher's law describes reliably (and with high accuracy) many data related to the electrode polarization phenomenon.

References


The study of adsorbed water in natural clays by dielectric spectroscopy

M.A. Vasilyeva¹, Yu.A. Gusev¹, V.G. Shtyrlin²

¹Institute of Physics, Kazan Federal University, 420008, Kremlyovskaya St., 18, Kazan, Russia.
²A.M. Butlerov Chemistry Institute, Kazan Federal University, 420008, Kremlyovskaya St., 18, Kazan, Russia.
e-mail: mariavasilyeva@mail.ru

The layer aluminosilicates (clay minerals) are the most widespread chemical compounds in the earth. The high specific surface area, chemical and mechanical stability, variety of structural and surface properties, higher values of cation exchange capacities, etc., make the clay minerals an excellent group of adsorbents. The electrical and adsorptive properties of the clay-water interface are of primary importance and used in fields such as pharmaceuticals, ecology, hydrogeology, agricultural chemistry, catalysis, petroleum, etc. Thus, obtaining an extensive and accurate knowledge about interaction between water molecules and surface of kaolinites and montmorillonites as typical representatives of natural layer aluminosilicates is an actual goal.

Dielectric spectroscopy was applied to natural clay minerals - montmorillonite with the exchangeable K⁺, Co²⁺, Ni²⁺, and Cu²⁺ cations and kaolinite with the exchangeable Na⁺, Mg²⁺, and Cu²⁺ cations, where the effect of water adsorption in the samples on the dielectric response was examined over wide temperature (-115 °C ÷ +300 °C) and frequency (1 Hz ÷ 1 MHz) ranges. All the samples were stored in ambient air humidity. In all the samples studied the complex non-Debye dielectric behavior was observed. Obtained dielectric spectra can be described in terms of distributed relaxation processes separated by different frequency and temperature ranges.

In present study we discussed the relaxation processes only at low and mid-temperatures. At low temperatures from -115 °C to – 75 °C the spectra of montmorillonites consist low and high frequency relaxation processes. Both these processes have strong temperature dependence. Such processes did not observed for kaolinites. In the mid-temperatures from –50 °C to +120 °C two relaxation processes having a specific saddle-like shape with distinctive kink point were observed for montmorillonite clays at different frequency-temperature intervals, while only one relaxation process was observed in the kaolinite samples.

The main features of water adsorption on the dielectric response of the natural clays are discussed. Comparison analysis of distributed relaxation processes allowed to understand the influence of the nature of the hydration centers on adsorbed water dynamics. Influence of exchangeable ions nature on the activation energy values of the relaxation processes is discussed.
Rotational dynamics of copper(II) amino acid complexes by EPR and NMR relaxation methods

M.S. Bukharov1,2), V.G. Shtyrlin1), G.V. Mamin1), A.S. Mukhtarov1), E.M. Gilyazetdinov1)

1) Kazan Federal University, A.M. Butlerov Chemistry Institute, 420008, Kremlevskaya St. 18, Kazan, Russian Federation.
2) Kazan Federal University, Institute of Physics, 420008, Kremlevskaya St. 18, Kazan, Russian Federation.
e-mail: mikhail.bukharov@gmail.com

Investigation of dynamical behavior of molecules in solutions is very important fundamental problem of physics and chemistry of condensed matter. The reason of interest is lack of complete understanding of molecular dynamics depending on solvent nature, structure, and properties of the molecules. Also investigations of rotational dynamics in solutions draw big attention because rotation of molecules and their fragments often determine the ways and effectiveness of chemical reactions.

In this work dynamical behavior of the copper(II) amino acid bis-complexes in aqueous medium was studied by EPR and NMR relaxation methods. Copper(II) complexes with amino acids model many proteins and metal enzymes and serve as transport forms of copper in living cells so their investigation induces additional significant theoretical and practical interest in terms of understanding of living systems.

EPR spectra of the studied compounds were registered in the temperature range 278-320 K and simulated by the Easyspin program [1]. In the simulation the Wilson-Kivelson theory [2, 3] for fast motion was used to describe linewidths and to obtain rotational correlation times (\(\tau_R\)) of the complexes.

The frequency and temperature dependences of spin-lattice (\(T_1\)) and spin-spin (\(T_2\)) relaxation times of solvent protons were measured in solutions of the copper(II) complexes. The modified Solomon-Bloembergen-Morgan equations [4] taken into account g-tensor anisotropy of complexes were used to describe the experimental data. The main paramagnetic contribution to the observed relaxation times is due to relaxation of the axial coordinated water molecules of the complexes which exchange rapidly with other molecules in solution [5]. So from NMR relaxation data the rotational correlation times, activation energies of rotational motion, and the water proton – copper(II) distances were obtained and analyzed in dependence on amino acids nature and complexes structure.

Comparison of rotational correlation times reveals significant differences in values obtained by two methods (EPR and NMR relaxation) for the same complexes. Accounting of second sphere and outer sphere contributions to calculation of NMR relaxations data didn’t result in significant improvements. Possible reasons of these \(\tau_R\) discrepancies are considered.

References

New program for computation of the thermodynamic, spectral, and NMR relaxation parameters of coordination compounds in complex systems

Kazan Federal University, A.M. Butlerov Chemistry Institute, 420008, Kremlevskaya St. 18, Kazan, Russian Federation.
e-mail: akrutiko@ksu.ru

Determination of thermodynamic and kinetic parameters of equilibria and spectral characteristics of coordination compounds in solutions of complex systems is an important problem of coordination and physical chemistry that can not be resolved without a computer simulation. In most of the programs intended for these purposes only one additive physico-chemical response depending on the values of pH or concentrations of components of the equilibrium system is modeled. In this paper a new approach, providing a direct calculation of equilibrium constants, parameters of the chemical exchange reactions, and spectral characteristics of complexes on the base of data of several methods, including pH-potentimetry, multiwavelength electronic spectroscopy, and NMR relaxation, within a single computer program was proposed. The new approach is implemented in the program STALABS.

The STALABS program contains modern algorithms for non-linear function minimization such as subspace trust-region method based on the interior-reflective Newton method or singular Jacobian decomposition. Following the MCR-ALS program [1] we use FNNLS algorithm [2] to resolve pure electronic absorption spectra from spectral data and known concentration profiles. The STALABS has some advantages against other programs created in Kazan State University earlier for the analogous purposes — CPESSP [3] and STABLAB [4]. The program was written in cross-platform development environment and equipped with easy-to-use GUI interface.

Application of the STALABS program was demonstrated on the example of investigation of the complex nickel(II) - L/DL-histidine systems by joint usage of the pH-potentiometry, multiwavelength spectrophotometry, and NMR relaxation methods. A significant stereoselectivity of the opposite signs in the formation constants of the complexes Ni(His)(HisH)+ and Ni(His)2 with domination of meso-form in the latter case was indicated. Stereoselective effects in the electronic absorption spectra of the mentioned complexes were determined for the first time. Structural interpretation of the found stereoselective effects with respect to data of quantum-chemical computations is presented.

References
Application of the statistics of the fractional moments for correlation analysis of X-ray diffraction spectra
R.R Nigmatullin\textsuperscript{(1)}, A.E. Lipacheva\textsuperscript{(1)}

\textsuperscript{(1)}Institution of Physics, Kazan (Volga Region) Federal University, 420008, 18 Kremlyovskaya st., Kazan, Russian Federation.
e-mail: sasha.lipacheva@gmail.com

X-ray diffraction analysis is the most widespread method of identification of chemical combinations in patterns. Nowadays we know a lot of methods of quantitative phase analysis, but these methods require some additional experiments and generally are not reliable. The way of simplification of qualitative phase analysis problem is considered. This way is based on preliminary statistical treatment procedure of X-ray spectra. In this case the statistical approach means the analysis of X-ray spectra about their statistical proximity. It allows to select reliably enough patterns of identical phase structure. If we have such information, it is enough to carry out the qualitative phase analysis with only one of set of identical patterns.

The method of correlation analysis is considered in frameworks of the statistics of the fractional moments [1]. The statistics of the fractional moments based on generalization of statistics of the integer moments. It uses as an additional source of information all set of moments, including their integer and fractional values. The method includes following stages: (i) smoothing procedure (ii) calculation of external correlation of spectra (iii) calculation of internal correlation of spectra (iii) final analysis of statistical proximity of spectra.

The calculation of external correlation is made by analysis generalized mean value functions
\[ GMV_p = \left( \frac{1}{N} \sum_{i=1}^{N} |y_i|^p \right)^{1/p} \]
for compared spectra. It is necessary to plot GMV-functions for compared data sequences in moment space and make linear approximation of the received set of points. The value \( \alpha = k - 1 \), where \( k \) – the angular factor of the received straight line is the measure of external correlation. In a limiting case \( \alpha = 0 \).

For calculation internal correlation the generalized Pearson correlation function
\[ F_p = \frac{G_p(1,2)}{\sqrt{G_p(1,1)G_p(2,2)}}, \quad G_p(k,l) = \left( \frac{1}{N} \sum_{i=1}^{N} \frac{y_i^{(k)} y_i^{(l)}}{y_{\text{max}}^{(k)} y_{\text{max}}^{(l)}} \right)^{1/p} \]
is used. Analysis of this function allows to allocate the band of correlations in a moment space. The width of a band (in a limiting case equals to 1) is the measure of internal correlations.

For smoothing of spectra the procedure of optimal linear smoothing is used [2].

The described method was applied to processing of spectra of breeds-collectors one of the chinks of Lebedinsky’s oilfield. Samples with identical phase structure have been allocated and comparison with results of the classical phase analysis shows a good agreement.

References

Heat Capacity Anomalies In Liquid Crystals

D. Lukashenko1), B. Khasanov1)

1) Theoretical Physics Department, Institute of Physics, Kazan university, 420008, Kremlevskaya, 18, Kazan, Russia
e-mail: Shadow-LD@yandex.ru, bulat.khasanov@ksu.ru

The purpose of the present work is to explain the anomalous heat capacity near the weak first order nematic-isotropic phase transition in liquid crystal MBBA (methoxybenzilidenebutylaniline). The analysis of the temperature dependence of the specific heat shows that the fluctuations of the multicomponent order parameter in the Landau-de-Gennes model are not small both above and below of transition point.

In isotropic phase the theory agrees with the experiment results numerically.

In the nematic phase such a satisfying description of the experimental data cannot be attained although research has shown that the relative contributions of longitudinal and biaxial fluctuations of the order parameter have a considerable influence on specific heat near to transition temperature.

Using experimental values of temperature dependence of the order parameter allows the experimental data for MBBA to come into concurrence with our calculated heat capacity expressions as shown at Fig 1.

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Nonextensivity of superfluid at nanoscale

Y.V. Lysogorskiy\(^1\), D.A. Tayurskii\(^1\)

\(^1\)Institute of Physics, Kazan Federal University, 420008, 18, Kremlevskaya, Kazan, Russia.

e-mail: yura.lysogorskiy@gmail.com

The complex behavior of such quantum fluids like liquid \(^4\)He and liquid \(^3\)He in nanoporous media is determined by influence of randomly distributed geometrical confinement as well as by significant contribution from the surface atoms \([1,2]\). Such a complex interaction could lead to the nonextensivity of energy and entropy. In the present work we demonstrate the nonextensivity for superfluid at nanoscale. The system was modelised by means of density functional theory for superfluid helium \([3]\), because such approach could provide excitation spectrum of quasiparticles in a semiempirical way.

References
